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BIQUADRATIC SPLINE SMOOTHING MEAN VALUES

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Abstract

The notion of natural biquadratic spline is remembered and then it is used for the construction of the biquadratic spline smoothing given mean values (local integrals) on the rectangular grid. The algorithm for computing mean values of the smoothing spline (and then remaining needed local parameters of the spline) is described.

Key words: splines, biquadratic splines, smoothing splines

MS Classification: 41A15, 65D05

1 Statement of the problem

Let us have the rectangle $D = \langle a, b\rangle \times \langle c, d\rangle = \cup D_{ij}$ in the (x, y)-plane with the rectangular mesh

$$(\Delta) = (\Delta x) \times (\Delta y) = \{(x_i, y_j);\ i = 0(1)n+1,\ j = 0(1)m+1\}\ ,$$

$$(\Delta x) \equiv a = x_0 < x_1 < \cdots < x_n < x_{n+1} = b\ ,$$

$$(\Delta y) \equiv c = y_0 < y_1 < \cdots < y_m < y_{m+1} = d\ .$$

Definition 1 We call a biquadratic spline on (Δ) a function $s(x, y)$ with the properties:

1° $s(x, y) \in \mathbb{C}^{1,1}(D)$ (continuous first derivatives)

2° $s(x, y)$ is a biquadratic polynomial on each subrectangle $D_{ij} = \langle x_i, x_{i+1}\rangle \times \langle y_j, y_{j+1}\rangle$.

Let us denote $\mathbb{S}\,(\Delta)$ the linear space of such splines; there is

$$\dim \mathbb{S}\,(\Delta) = (n+3)\cdot(m+3)$$

(see [1], [2]).

Given further the values $\{g_{ij};\ i = 0(1)n+1,\ j = 0(1)m+1\}$, we call $s(x,y) \in \mathbb{S}\,(\Delta)$ *the spline interpolating given mean values* g_{ij}, if

$$g_{ij} = \frac{1}{h_i k_j} \iint\limits_{D_{ij}} s(x,y)\, dx dy \,,$$
$$h_i = x_{i+1} - x_i,\ k_j = y_{j+1} - y_j, \qquad i = 0(1)n,\ j = 0(1)m\,. \tag{1}$$

To determine such a spline uniquely, we have to prescribe e.g. boundary conditions. The algorithm for computing suitable local parameters

$$\text{(SG)} \qquad s_{ij},\ s_{i+1,j},\ s_{i,j+1},\ s_{i+1,j+1},\ g_{ij},\ g^x_{ij},\ g^x_{i,j+1},\ g^y_{ij},\ g^y_{i+1,j} \tag{2}$$

with

$$s_{ij} = s(x_i, y_j), \quad g^x_{ij} = \frac{1}{h_i} \int\limits_{x_i}^{x_{i+1}} s(x, y_j) dx, \quad g^y_{ij} = \frac{1}{k_j} \int\limits_{y_j}^{y_{j+1}} s(x_i, y) dy$$

for $s \in \mathbb{S}\,(\Delta)$ under proper boundary conditions is given in [2].
There are also mentioned another possible local representations (Taylor coefficients, (SD)-representation using values of the spline and some of its derivatives at the vertices of D_{ij}).

The natural biquadratic spline was stated there to be $s(x,y) \in \mathbb{S}\,(\Delta)$ with boundary conditions

$$s^{1,0}(x_0, y) \equiv s^{1,0}(x_{n+1}, y) \equiv s^{0,1}(x, y_0) \equiv s^{0,1}(x, y_{m+1}) \equiv 0 \tag{3}$$

and thatwise $s^{1,1}(x,y) \equiv 0$ on the whole boundary ∂D; it is uniquely determined by the values $\{g_{ij}\}$ and it minimizes the functional

$$J_1(f) = \|f^{1,1}\|_2^2 = \iint\limits_{D_{ij}} [f^{1,1}(x,y)]^2\, dx dy \tag{4}$$

(which represents some measure of "flatness" of the surface described by the function $f(x,y)$) on the class

$$\mathbb{V} = \{f \in W_2^{1,1}(D);\ h_i k_j g_{ij} = \iint\limits_{D_{ij}} f(x,y)\, dx dy;\ i = 0(1)n,\ j = 0(1)m\}\,.$$

Let us introduce two another functionals

$$J_2(f) = \sum_{i=0}^{n}\sum_{j=0}^{m} w_{ij}\left[h_i k_j p_{ij} - \iint\limits_{D_{ij}} f(x,y)\,dxdy\right]^2 \quad (5)$$

$$J(f,\alpha) = J_1(f) + \alpha\, J_2(f) \quad (6)$$

with given data $\{p_{ij}, w_{ij} \geq 0;\ \ i = 0(1)n,\ j = 0(1)m;\ \alpha > 0\}$.

The functional $J_2(f)$ evaluates "mean square deviation" of the mean values p_{ij} and the functional $J(f,\alpha)$ represents some compromise between "flatness" of the surface $f(x,y)$ and interpolation of mean values p_{ij}, controlled by means of the parameter α.

We seek for the function $f \in W_2^{1,1}(D)$ which gives the minimum to the functional $J(f,\alpha)$.

Theorem 1 *Let $D, (\Delta), \{p_{ij}\}, \{w_{ij}\}$, $\alpha > 0$ be given. The functional $J(f,\alpha)$ attains its minimum on $W_2^{1,1}(D)$ in some natural biquadratic spline $s \in \mathbb{S}\,(\Delta)$.*

Proof Let the minimum of $J(f,\alpha)$ is attained in some function $g \in W_2^{1,1}$ with mean values

$$g_{ij} = \frac{1}{h_i k_j}\iint\limits_{D_{ij}} g(x,y)\,dxdy\ .$$

Let us denote by $s(x,y)$ the natural biquadratic spline interpolating the same mean values g_{ij}. We have then $J_2(s) = J_2(g)$. But according to the extremal property of natural spline (see (3), [2]) there is $J_1(s) \leq J_1(g)$ and therefore $J(s,\alpha) \leq J(g,\alpha)$.

Definition 2 The natural spline minimizing $J(f,\alpha)$ we shall call "biquadratic spline smoothing mean values p_{ij}".

2 Parameters of the smoothing spline

We shall search now for the local parameters of the smoothing spline. Let us remember that its mean values g_{ij} are in general different from given values p_{ij}; the corresponding boundary conditions were recalled in (3). Our aim will be to express $J(s,\alpha)$ in some adequate local parameters and to compute their values from the condition of minima.

2.1 Let us start with the functional $J_1(s)$. Using Simpson's rule and bilinearity of $s^{1,1}$ in D_{ij} we have

$$J_1(s) = \iint\limits_{D} \left[s^{1,1}(x,y)\right]^2 dxdy = \sum_{i=0}^{n}\sum_{j=0}^{m} F_1^{ij}\ ,$$

where

$$F_1^{ij} = \iint\limits_{D_{ij}} \left[s^{1,1}(x,y)\right]^2 dxdy =$$

$$= \int_{y_j}^{y_{j+1}} \frac{h_i}{6}\{[s^{1,1}(x_i,y)]^2 + 4[s^{1,1}(x_{i+\frac{1}{2}},y)]^2 + [s^{1,1}(x_{i+1},y)]^2\}\, dy =$$

$$= \frac{h_i}{3}\int_{y_j}^{y_{j+1}} \{[s^{1,1}(x_i,y)]^2 + s^{1,1}(x_i,y)s^{1,1}(x_{i+1},y) + [s^{1,1}(x_{i+1},y)]^2\}\, dy =$$

$$= \frac{1}{9}h_i k_j \{(s_{ij}^{1,1})^2 + (s_{i,j+1}^{1,1})^2 + (s_{i+1,j}^{1,1})^2 + (s_{i+1,j+1}^{1,1})^2 + s_{ij}^{1,1}s_{i,j+1}^{1,1} + \tag{7}$$

$$+ s_{i,j}^{1,1}s_{i+1,j}^{1,1} + s_{i+1,j}^{1,1}s_{i+1,j+1}^{1,1} + s_{i,j+1}^{1,1}s_{i+1,j+1}^{1,1} + \frac{1}{2}s_{ij}^{1,1}s_{i+1,j+1}^{1,1} + \frac{1}{2}s_{i,j+1}^{1,1}s_{i+1,j}^{1,1}\}.$$

In the following we shall use the local parameters (SG) used in [2] for $s(x,y)$. The continuity conditions and boundary conditions for natural biquadratic spline can be expressed in matrix form as (see [2])

$$\mathbf{B}(\mathbf{G}^x)^T = 3\mathbf{C}\mathbf{G}^T, \qquad \mathbf{A}\mathbf{G}^y = 3\mathbf{D}\mathbf{G}, \qquad \mathbf{B}\mathbf{S}^T = 3\mathbf{C}(\mathbf{G}^y)^T \tag{8}$$

with matrices

$$\mathbf{G} = [g_{ij}]_{i,j=0}^{n,m}, \quad \mathbf{G}^x = [g_{ij}^x]_{i,j=0}^{n,m+1}, \quad \mathbf{G}^y = [g_{ij}^y]_{i,j=0}^{n+1,m}, \quad \mathbf{S} = [s_{ij}]_{i,j=0}^{n+1,m+1}$$

and tridiagonal regular $(n+2,n+2),(m+2,m+2)$-matrices

$$\mathbf{A} = \begin{bmatrix} 2\alpha_0 & \alpha_0 & & & \\ \alpha_0 & 2(\alpha_0+\alpha_1) & \alpha_1 & & \\ & \cdots\cdots & \cdots\cdots & \cdots\cdots & \\ & & \alpha_{n-1} & 2(\alpha_{n-1}+\alpha_n) & \alpha_n \\ & & & \alpha_n & 2\alpha_n \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} 2\beta_0 & \beta_0 & & & \\ \beta_0 & 2(\beta_0+\beta_1) & \beta_1 & & \\ & \cdots\cdots & \cdots\cdots & \cdots\cdots & \\ & & \beta_{m-1} & 2(\beta_{m-1}+\beta_m) & \beta_m \\ & & & \beta_m & 2\beta_m \end{bmatrix}, \tag{9}$$

where $\alpha_i = 1/h_i$, $\beta_j = 1/k_j$;
finally we denote by $\mathbf{D}$, $\mathbf{C}$ the $(n+2,n+1),(m+2,m+1)$-matrices

$$\mathbf{D} = \begin{bmatrix} \alpha_0 & & \\ \alpha_0 & \alpha_1 & \\ & \cdots\cdots & \\ & \alpha_{n-1} & \alpha_n \\ & & \alpha_n \end{bmatrix}, \qquad \mathbf{C} = \begin{bmatrix} \beta_0 & & \\ \beta_0 & \beta_1 & \\ & \cdots\cdots & \\ & \beta_{m-1} & \beta_m \\ & & \beta_m \end{bmatrix}. \tag{10}$$

We can write now directly the relations between matrices of parameters $\mathbf{G}^x$, $\mathbf{G}^y$, $\mathbf{S}$, and matrix $\mathbf{G}$ of data:

$$\begin{aligned}
\mathbf{G}^x &= 3\mathbf{G}\mathbf{C}^T\mathbf{B}^{-1}, \\
\mathbf{G}^y &= 3\mathbf{A}^{-1}\mathbf{D}\mathbf{G}\,, \\
\mathbf{S} &= 3\mathbf{G}^y\mathbf{C}^T\mathbf{B}^{-1} = 9\mathbf{A}^{-1}\mathbf{D}\mathbf{G}\mathbf{C}^T\mathbf{B}^{-1}\,.
\end{aligned} \tag{11}$$

To express the values of $J(s,\alpha)$ in parameters (2), we use relations (see [2]),

$$\begin{aligned}
s_{ij}^{1,1} &= \frac{4}{h_i k_j}\big[9g_{ij} - 3g_{i,j+1}^x - 3g_{i+1,j}^y + s_{i+1,j+1} - 6g_{ij}^x + \\
&\qquad + 2s_{i+1,j} - 6g_{ij}^y + 2s_{i,j+1} + 4s_{ij}\big], \\
s_{i+1,j}^{1,1} &= \frac{4}{h_i k_j}\big[-9g_{ij} + 3g_{i,j+1}^x + 6g_{i+1,j}^y - 2s_{i+1,j+1} + 6g_{ij}^x - \\
&\qquad - 4s_{i+1,j} + 3g_{ij}^y - s_{i,j+1} - 2s_{ij}\big], \\
s_{i,j+1}^{1,1} &= \frac{4}{h_i k_j}\big[-9g_{ij} + 6g_{i,j+1}^x + 3g_{i+1,j}^y - 2s_{i+1,j+1} + 3g_{ij}^x - \\
&\qquad - s_{i+1,j} + 6g_{ij}^y - 4s_{i,j+1} - 2s_{ij}\big], \\
s_{i+1,j+1}^{1,1} &= \frac{4}{h_i k_j}\big[9g_{ij} - 6g_{i,j+1}^x - 6g_{i+1,j}^y + 4s_{i+1,j+1} - 3g_{ij}^x + \\
&\qquad + 2s_{i+1,j} - 3g_{ij}^y + 2s_{i,j+1} + s_{ij}\big].
\end{aligned} \tag{12}$$

Substituing it into (7) we obtain

$$F_1^{ij} = \frac{4}{h_i k_j}\mathbf{v}^T M \mathbf{v}$$

with $\mathbf{v} = \big[g_{ij}, g_{i,j+1}^x, g_{i+1,j}^y, s_{i+1,j+1}, g_{ij}^x, s_{i+1,j}, g_{ij}^y, s_{i,j+1}, s_{i,j}\big]^T$ and symmetric matrix $\mathbf{M}$

$$\mathbf{M} = \begin{bmatrix}
36 & -18 & -18 & 9 & -18 & 9 & -18 & 9 & 9 \\
-18 & 12 & 9 & -6 & 6 & -3 & 9 & -6 & -3 \\
-18 & 9 & 12 & -6 & 9 & -6 & 6 & -3 & -3 \\
9 & -6 & -6 & 4 & -3 & 2 & -3 & 2 & 1 \\
-18 & 6 & 9 & -3 & 12 & -6 & 9 & -3 & -6 \\
9 & -3 & -6 & 2 & -6 & 4 & -3 & 1 & 2 \\
-18 & 9 & 6 & -3 & 9 & -3 & 12 & -6 & -6 \\
9 & -6 & -3 & 2 & -3 & 1 & -6 & 4 & 2 \\
9 & -3 & -3 & 1 & -6 & 2 & -6 & 2 & 4
\end{bmatrix}.$$

Using continuity conditions (8) and zero boundary conditions (3) for the natural spline $s(x,y)$, we obtain after some tedious manipulations

$$J_1(s) = \sum_{i=0}^{n}\sum_{j=0}^{m} \frac{36}{h_i k_j} g_{ij} \left[4g_{ij} - 2g^x_{i,j+1} - 2g^y_{i+1,j} + s_{i+1,j+1} - \right.$$

$$\left. - 2g^x_{ij} + s_{i+1,j} - 2g^y_{ij} + s_{i,j+1} + s_{ij}\right] . \qquad (13)$$

When we denote by $\mathbf{A}^x$, $\mathbf{A}^y$ the matrices with elements

$$\begin{aligned} a^x_{ij} &= (\mathbf{C}^T\mathbf{B}^{-1})_{ij} + (\mathbf{C}^T\mathbf{B}^{-1})_{i,j+1} , \qquad i,j = 0(1)m \\ a^y_{ij} &= (\mathbf{A}^{-1}\mathbf{D})_{ij} + (\mathbf{A}^{-1}\mathbf{D})_{i+1,j} , \qquad i,j = 0(1)n \end{aligned} \qquad (14)$$

and substitute (11) into (13) , we obtain then the explicit expression for $J_1(s)$ in parameters g_{ij}:

$$J_1(s) = 108 \sum_{i=0}^{n}\sum_{j=0}^{m} \frac{1}{h_i k_j} g_{ij} \left[\frac{4}{3} g_{ij} - 2\sum_{k=0}^{m} g_{ik} a^x_{kj} - 2\sum_{l=0}^{n} a^y_{il} g_{lj} + \right.$$

$$\left. + \sum_{k=0}^{m}\sum_{l=0}^{n} a^y_{il} g_{lk} a^x_{kj}\right] = F_1(\mathbf{G}) . \qquad (15)$$

2.2 For the second component $J_2(s)$ of $J(s,\alpha)$ we have

$$J_2(s) = \sum_{i=0}^{n}\sum_{j=0}^{m} w_{ij} h_i k_j [p_{ij} - g_{ij}]^2 , \qquad (16)$$

which is directly the function of parameters g_{ij} : $J_2(s) = F_2(\mathbf{G})$. Altogether we have

$$J(s,\alpha) = J_1(s) + \alpha\, J_2(s) = F_1(\mathbf{G}) + \alpha\, F_2(\mathbf{G}) =: F(\mathbf{G},\alpha) .$$

The necessary condition for $\mathbf{G}$ to be a point of minima is

$$\frac{\partial F(G)}{\partial g_{uv}} = \frac{\partial F_1(G)}{\partial g_{uv}} + \alpha \frac{\partial F_2(G)}{\partial g_{uv}} = 0 . \qquad (17)$$

Computing the partial derivatives, we obtain

$$\frac{\partial F_1(G)}{\partial g_{uv}} = \frac{288}{h_u k_v} g_{uv} - \frac{216}{h_u} \sum_{j=0}^{m} g_{uj} \left[\frac{1}{k_v} a^x_{jv} + \frac{1}{k_j} a^x_{vj}\right] + \qquad (18)$$

$$- \frac{216}{k_v} \sum_{i=0}^{n} g_{iv} \left[\frac{1}{h_u} a^y_{ui} + \frac{1}{h_i} a^y_{iu}\right] + 324 \sum_{j=0}^{m}\sum_{i=0}^{n} g_{ij} \left[\frac{1}{h_u k_v} a^y_{ui} a^x_{jv} + \frac{1}{h_i k_j} a^y_{iu} a^x_{vj}\right],$$

$$\frac{\partial F_2(G)}{\partial g_{uv}} = w_{uv} h_u k_v \left[g_{uv} - p_{uv}\right] . \qquad (19)$$

After substitution into (17) and some algebraic manipulations we obtain the system for computing mean-values of the smoothing spline, declared in the following theorem.

Theorem 2 *Let the mean-values p_{ij}, weight coefficients $w_{ij} \geq 0$, $i = 0(1)n$, $j = 0(1)m$ and parametr $\alpha > 0$ be given on the rectangular domain $D = \cup D_{ij}$ with the mesh (Δ).*

The biquadratic spline minimizing the functional $J(f, \alpha)$ given in (6) attains the mean-values $\{g_{ij},\ i = 0(1)n,\ j = 0(1)m\}$ which satisfy the system of linear equations

$$\frac{4}{3}\alpha_u\beta_v g_{uv} - \alpha_u \sum_{j=0}^{m} g_{uj}\left[\beta_v a^x_{jv} + \beta_j a^x_{vj}\right] - \beta_v \sum_{i=0}^{n} g_{iv}\left[\alpha_u a^y_{ui} + \alpha_i a^y_{iu}\right] +$$

$$+\frac{3}{2}\sum_{j=0}^{m}\sum_{i=0}^{n} g_{ij}\left[\alpha_u\beta_v a^y_{ui}a^x_{jv} + \alpha_i\beta_j a^y_{iu}a^x_{vj}\right] + \frac{1}{216}\alpha_u w_{uv} h_u k_v (g_{uv} - p_{uv}) = 0$$

$$u = 0(1)n, \quad v = 0(1)m\ ; \qquad (20)$$

where $\alpha_i = 1/h_i$, $\beta_j = 1/k_j$ and matrices $\mathbf{A}^x$, $\mathbf{A}^y$ are defined in (14).

3 Description of the algorithm BSSMV

Let the rectangle domain D with the knot set $(\Delta) = (\Delta x) \times (\Delta y)$ and data $\{p_{ij}, w_{ij};\ i = 0(1)n,\ j = 0(1)m\}$, $\alpha > 0$ be given.

1° Compute stepsizes h_i, k_j and nonzero arrays of the matrices **A**, **B**, **C**, **D** defined in (9)–(10).

2° Compute inverse matrices $\mathbf{A}^{-1}$, $\mathbf{B}^{-1}$ (full matrices).

3° Compute the coefficients of matrices $\mathbf{A}^x$, $\mathbf{A}^y$ defined in (14).

4° Calculate the coefficients of the matrix and the right-hand side of the system of equations (20).

5° Solve the system (20) for the mean-values g_{ij} of the smoothing spline $s(x, y)$.

6° Choose the local representation of the smoothing spline (according to the output needs) and compute the needed local parameters—e.g. from the continuity conditions (8) for the (SG)-representation

$$s(x,y) = (1-u)(1-v)(1-3u-3v+9uv)s_{ij} + u(1-v)(-2+3u+6v-9uv)s_{i+1,j} +$$
$$+ (1-u)v(-2+6u+3v-9uv)s_{i,j+1} + uv(4-6u-6v+9uv)s_{i+1,j+1} +$$
$$+ 6(1-u)(1-v)[u(1-3v)g^x_{ij} + v(1-3u)g^y_{ij}] + 6uv[(1-u)(3v-2)g^x_{i,j+1} +$$
$$+ (1-v)(3u-2)g^y_{i+1,j}] + 36u(1-u)v(1-v)g_{ij}\ ,$$

where $u = (x - x_i)/h_i$, $v = (y - y_j)/k_j$ in D_{ij}.

We can compute needed local parameters for another possible local representations (Taylor coefficients, function and partial derivatives values for (SD)-representation) using relations given in [2]. They need usually more storage capacity as the consequence of nonsymmetry of parameters placing.

Remark 1 On the contrary to the algorithms for bivariate interpolatory splines on rectangles (see e.g. [1], [4]) this algorithm does not result in splitting to repeated use of one-dimensional algorithms. Different approach resulting in repeated use of one-dimensional algorithms will be described in the following paper [3].

Remark 2 The continuous dependence of the resulting smoothing spline on the regulating parameter α in the functional $J(s,\alpha)$ allows us to regulate the degree of the compromise between two limiting cases:

a) for $\alpha \to 0_+$ the smoothing spline converges to natural biquadratic spline with $s^{1,1}(x,y) \equiv 0$ on D—to some smoothing plane;

b) for $\alpha \to +\infty$ the minimizing property results in the convergence of the smoothing spline to the natural spline interpolating the given mean-values p_{ij}.

4 Examples

Example 1 Let $D = [0,2] \times [0,2]$, $(\Delta x) \equiv \{0,1,2\}$, $(\Delta y) \equiv \{0,1,2\}$,

$$\mathbf{G} = \begin{bmatrix} 2 & 1 \\ 1 & 0 \end{bmatrix}, \qquad [w_{ij}] = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}.$$

We can see the spline interpolating the given mean-values under zero boundary conditions (one-dimensional mean-values, function values at vertices) on Fig. 1.

Fig. 2 shows the smoothing spline for $p_{ij} = g_{ij}$ and $\alpha = 100$. Here

$$\mathbf{S} = [s_{ij}] = \begin{bmatrix} 2.5 & 1.75 & 1 \\ 1.75 & 1 & 0.25 \\ 1 & 0.25 & -0.5 \end{bmatrix}.$$

Example 2 Let $D = [-2,1] \times [-2,1]$, $(\Delta x) \equiv \{-2,-0.5,0,0.5,1\}$, $(\Delta y) \equiv \{-2,0,1\}$,

$$\mathbf{G} = \begin{bmatrix} 3 & 2 \\ 0 & 1 \\ 1 & 2 \\ 1 & 0 \end{bmatrix}, \qquad \mathbf{P} = \begin{bmatrix} 2.98 & 2.04 \\ 0.05 & 0.9 \\ 1.09 & 1.82 \\ 0.91 & 0.18 \end{bmatrix}, \qquad \alpha = 50.$$

Fig. 3 shows the interpolating spline under boundary conditions $\{g^x_{ij}, g^y_{ij}, s_{ij}$ all equal to one $\}$.

On Fig. 4 we can see the smoothing spline corresponding to $\alpha = 50$ for perturbed data $\mathbf{P}$ and $w_{ij} \equiv 1$.

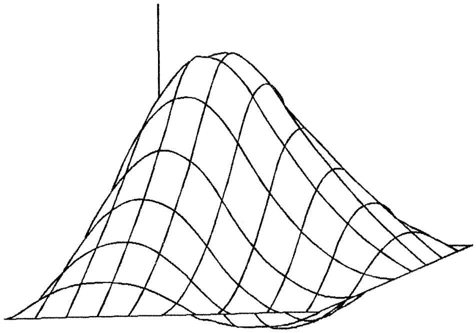

Fig. 1

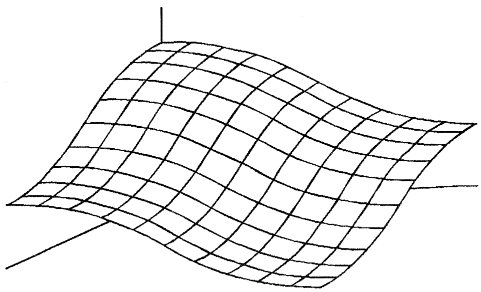

Fig. 2

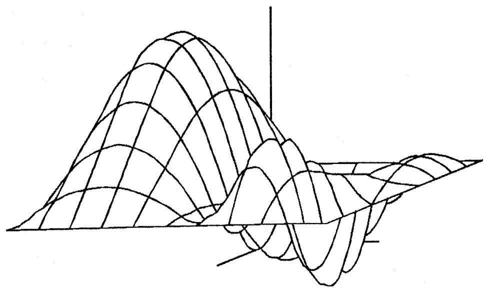

Fig. 3

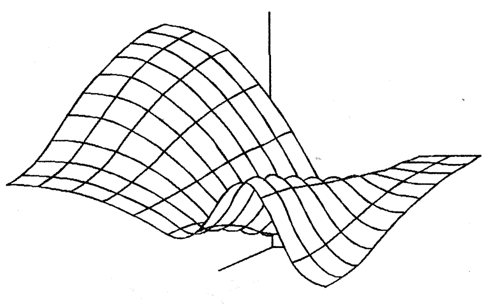

Fig. 4

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