CONSTRUCTIVE THEORY OF FUNCTIONS'87

SOFIA, 1988

ON INTERPOLATION BY BIVARIATE QUINTIC SPLINES OF CLASS C^2

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1. Introduction. The aim of this paper is to construct C^2-surfaces interpolating to given function values f_i at discrete points $\underline{x}^i = (x_1^i, x_2^i)$, $i = 1,\cdots,V$ scattered throughout a region Ω in the plane. For this purpose, we employ bivariate piecewise quintic polynomials (or quintic **splines**), with respect to a **triangulation** of Ω having the data points $\underline{x}^i$ as its vertices.

There are essentially two different strategies to solve scattered data interpolation problems by globally twice differentiable splines over triangles. In order to enforce C^2-smoothness **locally**, the splines must be of a sufficiently high degree. Specifically, a **nonic** local spline interpolant of class C^2 has been proposed by Whelan [7]. This interpolant, however, has two drawbacks, namely (i) it is computationally uneconomical (due to the high degree), (ii) it requires derivative data through order four at the vertices (which is almost never available in practical applications). On the other hand, one may consider splines with **globally** enforced smoothness properties. Clearly, a necessary condition for interpolability is that the dimension of the interpolation space equals or exceeds the number of interpolation conditions. C^2-**quintics** provide sufficient degrees of freedom for interpolation (cf. Schumaker [6]) and are still computationally efficient.

2. Quintic splines of class C^2. In this section, we present an efficient **global representation** for a bivariate piecewise quintic interpolant of degree 5 and smoothness C^2 defined over a triangulation.

Suppose Ω is a simply connected polygonal domain in R^2. Let $\Delta = \{\Delta_j,\ j = 1,\cdots,T\}$ be a **triangulation** of Ω with data points $\underline{x}^i$ as vertices of the triangles Δ_j. It is understood that the intersection of two different triangles in Δ is either empty or equal to a common vertex or edge. Let V_0 and V_b, respectively, (with $V_0 + V_b = V$) denote the number of vertices in the interior and on the boundary of Ω. Let E_0 be the number of edges in the interior of Ω.

We now consider the space of all piecewise quintic polynomials of class C^2 over a triangulation Δ of Ω, i.e.

$$S_5^2(\Delta) = \{s \in C^2(\Omega) \mid s|_{\Delta_j} \in \Pi_5(\Delta_j) \ , \ j = 1,\cdots,T\} \ ,$$

where $\Pi_5(\Delta_j)$ is the linear space of quintic polynomials in two variables over Δ_j. The exact dimension of the space $S_5^2(\Delta)$ for arbitrary Δ is still an open problem. Thus far, only the following **lower bound** on its dimension has been found by Schumaker [6], namely $\dim S_5^2(\Delta) \geq \ell_b := 3(V + V_b + \sum_2 + 1) + \sum_3$, with $\sum_2$ (resp. $\sum_3$) the number of interior vertices where 2 (resp. 3) edges of **different** slope meet.

For practical applications, it is essential to obtain a suitable representation for splines in $S_5^2(\Delta)$. To this end, we first embed the space $S_5^2(\Delta)$ into a larger space with a simpler structure, i.e.

$$P_5^2(\Delta) = \{s \in C(\Omega) \mid s|_{\Delta_j} \in \Pi_5(\Delta_j) \ , \ j = 1,\cdots,T \ ; \ s \text{ is twice differentiable in all vertices of } \Delta\}.$$

Next, the splines in $P_5^2(\Delta)$ are constrained by certain smoothness conditions across the triangle edges in order to belong to the subspace $S_5^2(\Delta)$.

Let us review some notation utilized for representing bivariate piecewise polynomials. Let $\Delta_\ell = [i,j,k]$ be a triangle in Δ with vertices $\underline{x}^i$, $\underline{x}^j$ and $\underline{x}^k$. Any point $\underline{x} = (x_1,x_2)$ in Δ_ℓ can be expressed in terms of (nonnegative) **barycentric coordinates** $\lambda_i(\underline{x})$, $\lambda_j(\underline{x})$, $\lambda_k(\underline{x})$, such that

$$\underline{x} = \sum_{m=i,j,k} \lambda_m(\underline{x})\, \underline{x}^m \quad , \qquad \sum_{m=i,j,k} \lambda_m(\underline{x}) = 1 \ .$$

A **Bernstein polynomial** of degree 5 over Δ_ℓ is defined by

$$B_{\underline{\alpha}}(\underline{x}) = \frac{|\underline{\alpha}|!}{\alpha_1!\ \alpha_2!\ \alpha_3!} \lambda_i^{\alpha_1} \lambda_j^{\alpha_2} \lambda_k^{\alpha_3} \ , \quad |\underline{\alpha}| = \alpha_1 + \alpha_2 + \alpha_3 = 5 \ ,$$

where $\underline{\alpha} = (\alpha_1,\alpha_2,\alpha_3)$ is a multi-index in Z_+^3. There are precisely 21 distinct Bernstein polynomials of degree 5, which form a basis for $\Pi_5(\Delta_\ell)$. Thus, any bivariate quintic polynomial can be written in **Bézier-Bernstein** form

$$p(\underline{x}) = \sum_{|\underline{\alpha}|=5} b_{\alpha_1\alpha_2\alpha_3}\, B_{\underline{\alpha}}(\underline{x}).$$

The coefficients $b_{\alpha_1\alpha_2\alpha_3}$ are called Bézier **ordinates**, which can be associated with points $\frac{1}{5}(\alpha_1\underline{x}^i + \alpha_2\underline{x}^j + \alpha_3\underline{x}^k)$ in a mesh over Δ_ℓ (see Fig. 1a).

In order to parametrize splines in $P_5^2(\Delta)$ and to reduce the storage requirements of our interpolation scheme, we express some of the Bézier ordinates of $p(\underline{x})$ in terms of its **function values** $p(\underline{x}^m) = f_m$, **first order derivatives** $p_{x_1}(\underline{x}^m) = g_m$, $p_{x_2}(\underline{x}^m) = h_m$ and **second order derivatives** $p_{x_1x_1}(\underline{x}^m) = r_m$, $p_{x_1x_2}(\underline{x}^m) = s_m$, $p_{x_2x_2}(\underline{x}^m) = t_m$ at the triangle vertices $\underline{x}^m$, $m = i,j,k$. Therefore, we introduce the following notation

$$\underline{\gamma}_m = \nabla p(\underline{x}^m) = (g_m, h_m)^{\cdot}, \quad H_m = \nabla^2 p(\underline{x}^m) = \begin{pmatrix} r_m & s_m \\ s_m & t_m \end{pmatrix}$$

for the **gradient** and **Hessian**, respectively, of the quintic p at vertex $\underline{x}^m$. We denote multiples of the first and second order **directional** derivatives of p, in the direction of vectors

$$\underline{e}_1 = \underline{x}^j - \underline{x}^i, \quad \underline{e}_2 = \underline{x}^k - \underline{x}^j, \quad \underline{e}_3 = \underline{x}^i - \underline{x}^k$$

parallel to the edges of Δ_ℓ, by

$$d_n^m = \frac{1}{5}\underline{e}_n^T\underline{\gamma}_m, \quad D_{nq}^m = \frac{1}{20}\underline{e}_n^T H_m \underline{e}_q, \quad m = i,j,k, \quad n,q = 1,2,3 .$$

We can now write six of the Bézier ordinates in terms of function values and derivatives of p at vertex $\underline{x}^i$

$$b_{500} = f_i, \quad b_{410} = f_i + d_1^i, \quad b_{320} = f_i + 2d_1^i + D_{11}^i,$$
$$b_{311} = f_i + d_1^i - d_3^i - D_{13}^i, \quad b_{401} = f_i - d_3^i, \quad b_{302} = f_i - 2d_3^i + D_{33}^i$$

(similar expressions for $\underline{x}^j$ and $\underline{x}^k$ are easily obtained by symmetry). The bivariate quintic polynomial p requires 21 parameters for its definition, namely 6 parameters $\{f_m, g_m, h_m, r_m, s_m, t_m\}$ at each vertex $\underline{x}^m$, $m = i,j,k$ and the remaining 3 Bézier ordinates $b_1^{(\ell)} = b_{221}$, $b_2^{(\ell)} = b_{122}$, $b_3^{(\ell)} = b_{212}$ over Δ_ℓ. Since quintic polynomials on adjacent triangles depend on the **same** parameters associated with common **vertices**, the resulting piecewise quintic spline over Δ is not only continuous on Ω, but also twice differentiable at all vertices of Δ. Hence, every choice of the $6V + 3T$ parameters, arising from the entire triangulation Δ, determines a spline belonging to $P_5^2(\Delta)$. Indeed, it was shown by Alfeld [1] that the space $P_5^2(\Delta)$ is of dimension $6V + 3T$.

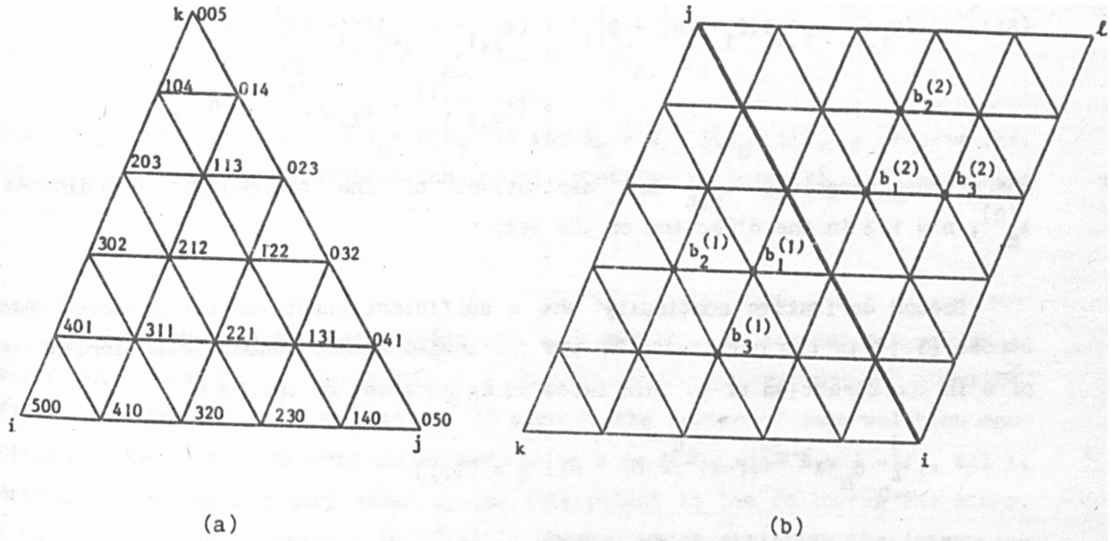


Fig. 1.

Now we impose smoothness constraints which force splines from $P_5^2(\Delta)$ into the subspace $S_5^2(\Delta)$. Suppose p_1 and p_2 are the quintic pieces of a spline s in $P_5^2(\Delta)$ on two adjacent triangles $\Delta_1 = [i,j,k]$ and $\Delta_2 = [i,j,\ell]$, respectively (see Fig. 1b). In order to simplify the notation, let $\underline{e}_4 = \underline{x}^\ell - \underline{x}^j$, $\underline{e}_5 = \underline{x}^i - \underline{x}^\ell$ and let $\lambda_m^{(n)}$, $b_q^{(n)}$ (q = 1,2,3) denote the barycentric coordinates and Bézier ordinates, respectively, associated with triangle Δ_n , n = 1,2.

First derivative continuity. The spline s will certainly be C^1-smooth across the common edge [i,j], if its first order derivative in the direction of any vector $\underline{\nu}$ (not parallel to $\underline{e}_1$) is continuous across [i,j]. Taking $\underline{\nu} = \underline{x}^\ell - \underline{x}^k$ and equating the (quartic) first order derivatives of p_1 and p_2 on [i,j] yields a condition of the form

$$\sum_{m=0}^{4} c_m \lambda^{4-m} (1-\lambda)^m = 0, \quad \text{all } \underline{x} \in [i,j],$$

with $\lambda(\underline{x}) \in [0,1]$ a local affine coordinate along [i,j] and c_m, m = 0,···,4 coefficients depending on the vertex parameters and Bézier ordinates. In other words, for C^1-smoothness we must require $c_m = 0$, for all m. The conditions for m = 0,1,3,4 are automatically satisfied, due to the common use of parameters associated with $\underline{x}^i$ and $\underline{x}^j$. Hence, the equation $c_2 = 0$ forms the first smoothness constraint (S1) across [i,j], which can be stated as follows (cf. Gmelig Meyling and Pfluger [2])

$$\text{(S1)} \quad (\tau_{i,1}-\tau_{i,2})(f_i+2d_1^i+D_{11}^i)+(\tau_{j,1}-\tau_{j,2})(f_j-2d_1^j+D_{11}^j)$$

$$+(\tau_{k,1}b_1^{(1)}-\tau_{\ell,2}b_1^{(2)})=0 \quad ,$$

where the constants $\tau_{m,n}$ are derivatives of the barycentric coordinates $\lambda_m^{(n)}$, $n = 1,2$ in the direction of the vector $\underline{\nu}$.

Second derivative continuity. Now a sufficient condition for C^2-smoothness across $[i,j]$ is the continuity of the (piecewise cubic) second order derivative of s in the direction of $\underline{\nu}$. This leads to an equation of the form

$$\sum_{m=0}^{3} d_m \lambda^{3-m}(1-\lambda)^m = 0, \quad \text{all } \underline{x} \in [i,j]$$

and hence $d_m = 0$, $m = 0,\cdots,3$. Analogously, the conditions for $m = 0,3$ are automatically satisfied. The remaining two smoothness constraints (S2,S3) across $[i,j]$ are thus $d_1 = d_2 = 0$, or equivalently

$$\text{(S2)} \quad (f_i+d_1^i)(\tau_{i,1}^2-\tau_{i,2}^2)+2(f_i+2d_1^i+D_{11}^i)(\tau_{i,1}\tau_{j,1}-\tau_{i,2}\tau_{j,2})$$

$$+(f_j-2d_1^j+D_{11}^j)(\tau_{j,1}^2-\tau_{j,2}^2)+2(f_i+d_1^i-d_3^i-D_{13}^i)\,\tau_{i,1}\tau_{k,1}$$

$$-2(f_i+d_1^i-d_5^i-D_{15}^i)\tau_{i,2}\tau_{\ell,2}+2(b_1^{(1)}\tau_{j,1}\tau_{k,1}-b_1^{(2)}\tau_{j,2}\tau_{\ell,2})$$

$$+(b_3^{(1)}\tau_{k,1}^2-b_3^{(2)}\tau_{\ell,2}^2)=0$$

and

$$\text{(S3)} \quad (f_j-d_1^j)(\tau_{j,1}^2-\tau_{j,2}^2)+2(f_j-2d_1^j+D_{11}^j)(\tau_{i,1}\tau_{j,1}-\tau_{i,2}\tau_{j,2})$$

$$+(f_i+2d_1^i+D_{11}^i)(\tau_{i,1}^2-\tau_{i,2}^2)+2(f_j-d_1^j+d_2^j-D_{12}^j)\tau_{j,1}\tau_{k,1}$$

$$-2(f_j-d_1^j+d_4^j-D_{14}^j)\tau_{j,2}\tau_{\ell,2}+2(b_1^{(1)}\tau_{i,1}\tau_{k,1}-b_1^{(2)}\tau_{i,2}\tau_{\ell,2})$$

$$+(b_2^{(1)}\tau_{k,1}^2-b_2^{(2)}\tau_{\ell,2}^2)=0\ .$$

We arrive at the conclusion that a spline s in $P_5^2(\Delta)$ is C^2-smooth throughout Ω, if the $6V + 3T$ parameters defining s satisfy $3E_0$ linear equations, namely (S1,S2,S3) for every **interior** edge in Δ. If we compute the remaining degrees of freedom

$$(6V + 3T) - 3E_0 = 3(V + V_b + 1) = \ell b - 3\sum_2 - \sum_3$$

(using Euler's formulas $T = V_b + 2(V_0 - 1)$ and $E_0 = V_b + 3(V_0 - 1)$), we observe that the linear system of smoothness constraints contains at least $3\sum_2 + \sum_3$ redundant equations.

3. Scattered data interpolation. In this section, we discuss a numerically efficient procedure for calculating a quintic spline interpolant of class C^2. Since the dimension of the space $S_5^2(\Delta)$ exceeds the number of interpolation conditions, there is in general no unique spline s in $S_5^2(\Delta)$ with $s(\underline{x}^i) = f_i$, all i. Hence, we determine a **particular** spline interpolant in the following two steps. First, a suitable function $\hat{s}$ in $P_5^2(\Delta)$ is chosen, which satisfies the interpolation conditions, but not necessarily the C^2-smoothness requirements. This is followed by the calculation of the final interpolant s from $S_5^2(\Delta)$, which (i) interpolates to the positional data f_i, (ii) is C^2-smooth throughout Ω and (iii) is, in some sense, as close as possible to $\hat{s}$ (cf. Grandine [4]).

initial interpolant $\hat{s}$

Since only function values f_i are given, reasonable estimates for the first and second order derivatives at the triangle vertices must be generated. In order to estimate derivatives from scattered positional data, Lawson [5] suggests to compute for every vertex $\underline{x}^i = (x_1^i, x_2^i)$ a **quadratic polynomial**

$$q_i(x_1,x_2) = f_i + \alpha_i(x_1 - x_1^i) + \beta_i(x_2 - x_2^i) + \frac{1}{2}\gamma_i(x_1 - x_1^i)^2$$

$$+ \delta_i(x_1 - x_1^i)(x_2 - x_2^i) + \frac{1}{2}\varepsilon_i(x_2 - x_2^i)^2 ,$$

which **interpolates** to f_i at data point $\underline{x}^i$ and **fits** to data f_j at a number of adjacent vertices $\underline{x}^j$ ($j \neq i$) in "inverse distance weighted" least squares sense. In other words the function q_i is the solution of the linear least squares problem

$$\underset{q_i}{\text{minimize}} \sum_{j \neq i} \left(\frac{q_i(\underline{x}^j) - f_j}{\text{dist}(\underline{x}^i, \underline{x}^j)} \right)^2 .$$

The coefficients of the quadratic function q_i then provide estimates for the derivatives, i.e. $g_i = \alpha_i$, $h_i = \beta_i$, $r_i = \gamma_i$, $s_i = \delta_i$, $t_i = \varepsilon_i$. Although there are many possible methods for choosing values of the Bézier ordinates $b_1^{(\ell)}$,

$b_2^{(\ell)}$, $b_3^{(\ell)}$, we employ a technique which reproduces **quadratics** exactly from discrete data. For instance, a suitable formula for the Bézier ordinate $b_1^{(\ell)}$, associated with a triangle $\Delta_\ell = [i,j,k]$, is

$$b_1^{(\ell)} = 12(f_i + f_j) + 6f_k + 15(d_1^i - d_1^j) + \frac{15}{2}(d_2^j - d_2^k + d_3^k - d_3^i)$$

(cf. Gmelig Meyling and Pfluger [2]).

C^2-smooth interpolant s

At this stage, the n_p (= 5V + 3T) parameters $\{g_i, h_i, r_i, s_i, t_i \; ; \; i = 1,\cdots,V\}$ and $\{b_1^{(\ell)}, b_2^{(\ell)}, b_3^{(\ell)} \; ; \; \ell = 1,\cdots,T\}$ of the interpolant $\hat{s}$ from $P_5^2(\Delta)$ will be adjusted slightly, in order to satisfy the restrictive C^2-smoothness constraints. Let us associate these parameters with a vector $\underline{\hat{v}}$ in R^{n_p}. It is our objective to compute a vector $\underline{v}$, whose components define s and satisfy the underdetermined linear system $A\underline{v} = \underline{b}$, arising from the n_c (= $3E_0$) smoothness conditions (S1,S2,S3) across the interior edges of Δ. Here, all terms involving given positional data f_i have been transferred to the right-hand side vector $\underline{b} \in R^{n_c}$. In general, the spline $\hat{s}$ will not be consistent with the C^2-smoothness requirements, i.e. $\underline{r} = \underline{b} - A\underline{\hat{v}} \neq \underline{0}$. Therefore, we calculate a **correction vector** $\underline{e}$ of **minimal 2-norm** as follows

(i) solve a vector $\underline{y} \in R^{n_c}$ from $AA^T \underline{y} = \underline{r}$,

(ii) set $\underline{e} = A^T\underline{y}$.

Obviously, the vector $\underline{v} = \underline{\hat{v}} + \underline{e}$ now satisfies all the conditions for C^2 smoothness (and thus s belongs to $S_5^2(\Delta)$), since

$$A\underline{v} = A(\underline{\hat{v}} + \underline{e}) = (\underline{b} - \underline{r}) + A(A^T\underline{y}) = (\underline{b} - \underline{r}) + \underline{r} = \underline{b} \; .$$

We point out that this method does not fail when applied to a matrix $A \in R^{n_c \times n_p}$ with rank(A) < n_c, e.g. in the case of a triangulation Δ where $3\sum_2 + \sum_3 > 0$. Computing the vector $\underline{y}$ amounts to solving a large, however sparse, linear system $AA^T\underline{y} = \underline{r}$ with a symmetric positive semi-definite coefficient matrix. This main computational task is accomplished with the aid of the **conjugate gradient** (CG) method (cf. Golub and van Loan [3]). This is an iterative method, which generates a sequence of approximations $\{\underline{y}^{(k)}\}$ converging to the vector $\underline{y}$. The CG-algorithm has low storage requirements and involves only two matrix-vector products per iteration.

The rate of convergence of the CG-method can be improved considerably by an acceleration technique, namely **incomplete Cholesky factorization** (see [3],

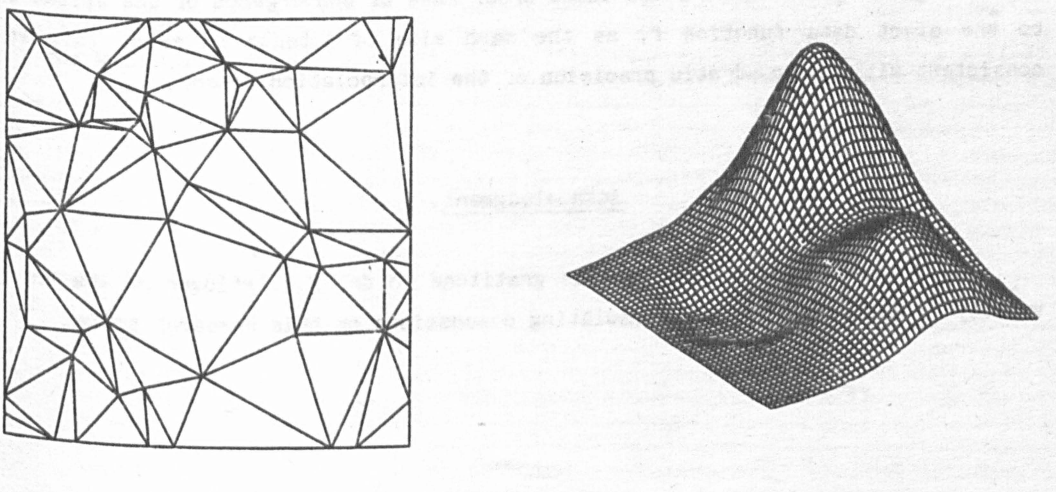
p. 376). To this end, one computes a nonsingular lower triangular matrix L, which is a suitable approximation to the exact Cholesky factor of AA^T (i.e. $LL^T \approx AA^T$). The idea behind this approach is that the matrix BB^T, with $B = L^{-1}A$, has improved condition. Therefore, the so-called **preconditioned** CG-algorithm is likely to obtain an accurate solution $\underline{z}$ to the transformed system $BB^T\underline{z} = L^{-1}\underline{r}$ in fewer iterations. The original vector $\underline{y}$ can then be solved from the triangular system $L^T\underline{y} = \underline{z}$. A suitable preconditioning strategy leads to very rapid convergence (often within far fewer than n_c iterations), at the expense of somewhat more work and storage per iteration. Finally, full advantage can be taken from the **sparsity** of the matrices A and L.

4. Numerical experiments. In this section, we present some numerical evidence that our scheme is of advantage for the solution of practical scattered data interpolation problems.

Consider the non-uniform triangulation Δ of the unit square displayed in Fig. 2a. This triangular mesh has the following characteristic properties

$$V = 62,\ V_b = 28,\ T = 94,\ E_0 = 127,\ \textstyle\sum_2 = 0,\ \sum_3 = 1.$$

It can be shown that the associated spline space $S_5^2(\Delta)$ is of dimension 274 (which equals the lower bound ℓb) by calculating the **singular value decomposition** of the constraint matrix A.



(a) (b)

Fig. 2.

The interpolation method is applied to data drawn from a well-known bivariate **test** function f, first introduced by Franke (cf. Whelan [7]). Suitable estimates for the derivatives of $\hat{s}$ at every data point $\underline{x}^i$ are generated by solving V linear least squares problems, taking positional data into account from eight adjacent vertices (including the immediate neighbours of $\underline{x}^i$). Next, the n_p (= 592) components of the vector $\underline{v}$ defining a C^2-smooth interpolating spline s are determined by the preconditioned CG-method. Only 189 iterations are required to solve the vector $\underline{z}$ from the linear system $BB^T\underline{z} = L^{-1}\underline{r}$ consisting of n_c (= 381) equations. Here, the solution is calculated to full relative machine accuracy, namely 10^{-12} on a VAX 8650-computer with double precision arithmetic. As a comparison, 1715 iterations would be necessary if no preconditioning is employed. The storage requirements of the algorithm are dominated by the number of nonzeros in A and L (5080 and 5573, respectively). The resulting interpolation errors over $[0,1]^2$

$$\frac{\|s-f\|_\infty}{\|f\|_\infty} = 0.098, \quad \frac{\|s_{x_1} - f_{x_1}\|_\infty}{\|f_{x_1}\|_\infty} = 0.83, \quad \frac{\|s_{x_2} - f_{x_2}\|_\infty}{\|f_{x_2}\|_\infty} = 0.82$$

give an impression of the (relative) accuracy of the piecewise quintic C^2-smooth interpolant s. Fig. 2b displays a perspective plot of the interpolating surface s, which is composed of 94 bivariate quintic polynomial pieces matching C^2-smoothly at the triangle edges.

Various numerical experiments with our algorithm for different data sets and triangular grids confirm the **third** order rate of convergence of the spline s to the exact data function f, as the mesh size of Δ tends to zero. This is consistent with the **quadratic precision** of the interpolation scheme.

Acknowledgment.

The author wishes to express his gratitude to dr. P.R. Pfluger of the University of Amsterdam for the stimulating discussions on this research topic.

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