Journal of Computational and Applied Mathematics 15 (1986) 161–173
North-Holland

An algorithm for fitting data over a circle using tensor product splines *

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Received 25 May 1984
Revised 20 February 1985

Abstract: An algorithm is described for surface fitting over a circle by using tensor product splines which satisfy certain boundary conditions. This algorithm is an extension of an existing one for fitting data over a rectangle. The knots of the splines are chosen automatically but a single parameter must be specified to control the tradeoff between closeness of fit and smoothness of fit. The algorithm can easily be generalized for fitting data over any domain that can be described in polar coordinates. Constraints at the boundaries of this approximation domain can be imposed.

1. Introduction

In [4], a semi-automatic algorithm is described for surface fitting with tensor product splines. Besides the set of data points, the user merely has to provide a parameter S, called 'the smoothing factor', by which he can control the trade-off between closeness of fit and smoothness of fit. The number of knots of the spline and their position are then determined automatically in an attempt to take account of the behaviour of the function underlying the data. The user must also specify a rectangular domain on which the approximation is determined. This can be rather inconvenient in applications with a well specified and nonrectangular approximation domain (e.g. the wing of an aeroplane on which a pressure distribution has to be approximated), especially if constraints at the boundary are to be satisfied.

In this paper we will therefore show how the surface fitting algorithm can be adapted for nonrectangular domains which can easily be described in polar coordinates. We begin by considering the unit disc $C = \{(x, y) \mid x^2 + y^2 \leqslant 1\}$. If a smooth function $F(x, y)$ on C is represented in polar coordinates, i.e. $f(u, v) = F(u \cos v, u \sin v)$, then this function f will satisfy certain boundary conditions on its domain $D = \{(u, v) \mid 0 \leqslant u \leqslant 1;\ -\pi \leqslant v \leqslant \pi\}$. In Section 2 we derive the conditions which guarantee C^2 continuity for F. How these can be incorporated in an elegant way, into a tensor product spline $s(u, v)$ on D, is explained in Section 3. In Section 4 we can then describe our adapted surface fitting algorithm. Finally in Section 5, we demonstrate how this algorithm can be generalized if we have an approximation domain C^* which can be described through a smooth periodic function $R(v)$, i.e. if $f(u, v) = F(uR(v) \cos v, uR(v) \sin v)$ on D. We also briefly discuss how we can impose additional constraints for F at the boundary of C^*.

* This research was supported by the FKFO under grant 2.0021.75.

In Section 6, some numerical results are presented, which were obtained from a Fortran program based on the algorithm described.

2. Continuity conditions

Let $F(x, y)$ be a smooth function with bounded derivatives on the unit disc C. Consider the mapping

$$x = u\cos v, \qquad y = u\sin v, \qquad 0 \leqslant u \leqslant 1, \quad -\pi \leqslant v \leqslant \pi. \tag{2.1}$$

Then $f(u, v) = F(x, y)$ is also smooth and has bounded derivatives on the rectangle $D = [0, 1] \times [-\pi, \pi]$. Additionally, f will satisfy some boundary conditions. It is necessary to know them because later they will be imposed upon a spline approximation s for f and ensure in this way that $S(x, y) = s(u, v)$ is also sufficiently smooth on C. We use bicubic splines. So, we will content ourselves with conditions which guarantee C^2 continuity.

First of all, f must be periodic in the variable v. Also

$$f(0, v) = F_{0,0}, \quad -\pi \leqslant v \leqslant \pi, \tag{2.2}$$

where we use the notation

$$F_{i,j} = \partial^{i+j} F(0, 0)/\partial x^i \partial y^j. \tag{2.3}$$

The existence of $F_{1,0}$ requires that

$$\frac{\partial f}{\partial u}(0, 0) = -\frac{\partial f}{\partial u}(0, \pi) = F_{1,0}. \tag{2.4}$$

Continuity of this derivative at the origin therefore means that

$$\lim_{(x,y)\to(0,0)} \frac{\partial F}{\partial x}(x, y) = \frac{\partial f}{\partial u}(0, 0). \tag{2.5}$$

From (2.1) we easily derive that

$$\frac{\partial F}{\partial x}(x, y) = \cos v \frac{\partial f}{\partial u}(u, v) - \frac{\sin v}{u}\frac{\partial f}{\partial u}(u, v), \quad (x, y) \neq (0, 0). \tag{2.6}$$

If we replace $\partial f/\partial u$ and $\partial f/\partial v$ (considered as functions of u) by their Maclaurin expansion and take account of the fact that $\partial f(0, v)/\partial v \equiv 0$ as follows from (2.2), condition (2.5) then simply becomes

$$\cos v \frac{\partial f}{\partial u}(0, v) - \sin v \frac{\partial^2 f}{\partial u \partial v}(0, v) = \frac{\partial f}{\partial u}(0, 0). \tag{2.7}$$

From the continuity of $\partial F/\partial y$ we obtain in a similar way that

$$\frac{\partial f}{\partial u}(0, \tfrac{1}{2}\pi) = -\frac{\partial f}{\partial u}(0, \tfrac{1}{2}\pi) = F_{0,1} \tag{2.8}$$

and

$$\sin v \frac{\partial f}{\partial u}(0, v) + \cos v \frac{\partial^2 f}{\partial u \partial v}(0, v) = \frac{\partial f}{\partial u}(0, \tfrac{1}{2}\pi). \tag{2.9}$$

Now, let

$$G(v)=\frac{\partial f}{\partial u}(0,\ v). \tag{2.10}$$

Then by differentiation (2.7) and (2.9) we find twice that

$$G''(v)+G(v)=0, \tag{2.11}$$

so that, taking account of the conditions (2.4) and (2.8) we may conclude that

$$\frac{\partial f}{\partial u}(0,\ v)=F_{1,0}\cos v+F_{0,1}\sin v,\quad -\pi\leqslant v\leqslant\pi. \tag{2.12}$$

In a similar way, we can find from the definition of the second order partial derivatives at the origin, that

$$\frac{\partial^2 f}{\partial u^2}(0,\ 0)=\frac{\partial^2 f}{\partial u^2}(0,\ \pi)=F_{2,0}. \tag{2,13}$$

$$\frac{\partial^2 f}{\partial u^2}(0,\ \tfrac{1}{2}\pi)=\frac{\partial^2 f}{\partial u^2}(0,\ \tfrac{1}{2}\pi)=F_{0,2}, \tag{2.14}$$

$$\frac{\partial^3 f}{\partial u^2\partial v}(0,\ 0)=\frac{\partial^3 f}{\partial u^2\partial v}(0,\ \pi)=-\frac{\partial^3 f}{\partial u^2\partial v}(0,\ \tfrac{1}{2}\pi)=-\frac{\partial^3 f}{\partial u^2\partial v}(0,\ \tfrac{1}{2}\pi)=2F_{1,1}. \tag{2.15}$$

Continuity of these derivatives yields the following differential equation

$$H'''(v)+4H'(v)=0 \tag{2.16}$$

for

$$H(v)=\frac{\partial^2 f}{\partial u^2}(0,\ v). \tag{2.17}$$

We may conclude therefore that

$$\frac{\partial^2 f}{\partial u^2}(0,\ v)=F_{2,0}\cos^2 v+F_{0,2}\sin^2 v+F_{1,1}\sin 2v. \tag{2.18}$$

We have also proved that the conditions (2.2), (2.12) and (2.18) are both necessary and sufficient.

3. Tensor product splines for the unit disc

Consider the rectangular domain $D=[0,\ 1]\times[-\pi,\ \pi]$ and the strictly increasing sequence of real numbers

$$0=\lambda_0<\lambda_1<\cdots<\lambda_g<\lambda_{g+1}=1, \tag{3.1}$$

$$-\pi=\mu_0<\mu_1<\cdots<\mu_h<\mu_{h+1}=\pi. \tag{3.2}$$

Then the function $s(u,\ v)$ is called a spline on D, of degree k in u and l in v, with knots λ_i, $i=1,2,\ldots,g$, in the u-direction and μ_j, $j=1,2,\ldots,h$, in the v-direction if the following conditions are satisfied:

(i) On any subrectangle $D_{i,j}=[\lambda_i,\ \lambda_{i+1}]\times[\mu_j,\ \mu_{j+1}]$, $i=0,\ldots,g$; $j=0,\ldots,h$, $s(u,\ v)$ is given by a polynominal of degree k in u and l in v.

(ii) All derivatives $\partial^{i+j}s(u, v)/\partial u^i \partial v^j$ for $0 \leqslant i \leqslant k-1$ and $0 \leqslant j \leqslant l-1$ are continuous in D.

If we introduce a number of additional knots satisfying

$$\lambda_{-k} \leqslant \lambda_{-k+1} \leqslant \cdots \leqslant \lambda_{-1} \leqslant 0, \quad 1 \leqslant \lambda_{g+2} \leqslant \cdots \leqslant \lambda_{g+k} \leqslant \lambda_{g+k+1}, \tag{3.3}$$

$$\mu_{-l} \leqslant \mu_{-l+1} \leqslant \cdots \leqslant \mu_{-1} \leqslant -\pi, \quad \pi \leqslant \mu_{h+2} \leqslant \cdots \leqslant \mu_{h+l} \leqslant \mu_{h+l+1}, \tag{3.4}$$

but which are otherwise arbitrary, every such spline on D can uniquely be expressed as

$$s(u, v) = \sum_{i=-k}^{g} \sum_{j=-l}^{h} c_{i,j} M_{i,k+1}(u) N_{j,l+1}(v), \tag{3.5}$$

where $M_{i,k+1}(u)$ and $N_{j,l+1}(v)$ are normalized B-splines [1]. These B-splines enjoy the following properties

$$M_{i,k+1}(u) = 0 \quad \text{if } u < \lambda_i \text{ or } u > \lambda_{i+k+1}, \tag{3.6}$$

$$M'_{i,k+1}(u) = k\left[\frac{M_{i,k}(u)}{\lambda_{i+k} - \lambda_i} - \frac{M_{i+1,k}(u)}{\lambda_{i+k+1} - \lambda_{i+1}}\right], \tag{3.7}$$

$$\sum_i M_{i,k+1}(u) \equiv 1, \tag{3.8}$$

and they can be evaluated in a very stable way using the recurrence scheme of de Boor [1] and Cox [2], i.e.

$$M_{i,k+1}(u) = \frac{u - \lambda_i}{\lambda_{i+k} - \lambda_i} M_{i,k}(u) + \frac{\lambda_{i+k+1} - u}{\lambda_{i+k+1} - \lambda_{i+1}} M_{i+1,k}(u), \tag{3.9}$$

$$M_{i,1}(u) = \begin{cases} 1 & \text{if } \lambda_i \leqslant u < \lambda_{i+1}, \\ 0 & \text{if } u < \lambda_i \text{ or } u \geqslant \lambda_{i+1}. \end{cases} \tag{3.10}$$

Analogous results apply to the B-splines $N_{j,l+1}(v)$.

From [4] we recall the conditions for $s(u, v)$ to be a single polynomial on D, i.e.

$$\sum_{i=-k}^{g} a_{i,q} c_{i,j} = 0, \qquad q = 1, 2, \ldots, g, \quad j = -l, -l+1, \ldots, h, \tag{3.11}$$

and

$$\sum_{j=-l}^{h} b_{j,r} c_{i,j} = 0, \qquad r = 1, 2, \ldots, h, \quad i = -k, -k+1, \ldots, g, \tag{3.12}$$

where the coefficients $a_{i,q}$ and $b_{j,r}$ denote the discontinuity jumps in the derivatives of the B-splines at the interior knots, i.e.

$$a_{i,q} = M^{(k)}_{i,k+1}(\lambda_q + 0) - M^{(k)}_{i,k+1}(\lambda_q - 0), \tag{3.13}$$

$$b_{j,r} = N^{(l)}_{j,l+1}(\mu_r + 0) - N^{(l)}_{j,l+1}(\mu_r - 0). \tag{3.14}$$

In our application we are interested in spline functions which are periodic in the variable v. If we choose the boundary knots (3.4) in the following way

$$\mu_{-j} = \mu_{h+1-j} - 2\pi, \quad \mu_{j+h+1} = \mu_j + 2\pi, \qquad j = 1, 2, \ldots, l, \tag{3.15}$$

then (see e.g. [5])

$$N_{-j,l+1}(v) \equiv N_{-j+h+1,l+1}(v + 2\pi), \quad j = 1, 2, \ldots, l. \tag{3.16}$$

Therefore, by taking account of property (3.6) and (3.7), applied to the B-splines $N_{j,l+1}(v)$, we find that

$$\frac{\partial^j s(u,-\pi)}{\partial v^j} \equiv \frac{\partial^j s(u,\pi)}{\partial v^j}, \qquad j=0,1,\ldots,l-1, \quad 0 \leqslant u \leqslant 1, \tag{3.17}$$

if the conditions

$$c_{i,h+1-j} = c_{i,-j}, \qquad i=-k,-k+1,\ldots,g, \quad j=1,2,\ldots,l, \tag{3.18}$$

are imposed. In Section 2 we find the other conditions for $S(x, y) = s(\sqrt{x^2+y^2}, \arctan(y/x))$ to have continuous second order derivatives at the origin. From (2.2), (2.12) and (2.18) we know that there should be numbers $S_{i,j} = \partial^{i+j}S(0, 0)/\partial x^i \partial y^j$ such that

$$s(0, v) \equiv S_{0,0}, \tag{3.19}$$

$$\frac{\partial s(0, v)}{\partial u} \equiv S_{1,0} \cos v + S_{0,1} \sin v, \quad -\pi \leqslant v \leqslant \pi, \tag{3.20}$$

$$\frac{\partial^2 s(0, v)}{\partial u^2} \equiv S_{2,0} \cos^2 v + S_{0,2} \sin^2 v + S_{1,1} \sin 2v. \tag{3.21}$$

If the boundary knots (3.3) are chosen to be coincident ($\lambda_{-k} = \cdots = \lambda_{-1} = 0$), then (see e.g. [3])

$$M_{i,k+1}(0) = \delta_{i,-k}, \tag{3.22}$$

with $\delta_{i,j}$ the Kronecker delta. Consequently, from (3.5) and (3.8), it follows that (3.19) is equivalent to

$$c_{-k,j} = S_{0,0}, \quad j=-l,\ldots,h. \tag{3.23}$$

Condition (3.20) cannot be fulfilled exactly. However, it can be satisfied approximately if we replace cos v and sin v by their periodic spline interpolants Co(v) and Si(v), i.e.

$$\mathrm{Co}(v) = \sum_{j=-l}^{h} \alpha_j N_{j,l+1}(v), \tag{3.24}$$

with

$$\mathrm{Co}(\mu_j) = \cos(\mu_j), \quad j=0,1,\ldots,h, \tag{3.25}$$

$$\alpha_{-j} = \alpha_{h+1-j}, \qquad j=1,2,\ldots,l, \tag{3.26}$$

and

$$\mathrm{Si}(v) = \sum_{j=-l}^{h} \beta_j N_{j,l+1}(v) \tag{3.27}$$

analogously.

From (3.5), (3.7) and (3.6) it follows that

$$\frac{\partial s(u, v)}{\partial u} = k \sum_{i=-k+1}^{g} \sum_{j=-l}^{h} \frac{c_{i,j} - c_{i-1,j}}{\lambda_{i+k} - \lambda_i} M_{i,k}(u) N_{j,l+1}(v), \tag{3.28}$$

and consequently from (3.22) and (3.23) that

$$\frac{\partial s(0, v)}{\partial u} = \frac{k}{\lambda_1} \sum_{j=-l}^{h} (c_{-k+1,j} - S_{0,0}) N_{j,l+1}(v). \tag{3.29}$$

Substituting (3.29) into (3.20) and replacing $\cos v$ and $\sin v$ by the splines (3.24) and (3.27), we then obtain

$$c_{-k+1,j} = S_{0,0} + \tilde{S}_{1,0}\alpha_j + \tilde{S}_{0,1}\beta_j, \quad j = -l, \dots, h, \tag{3.30}$$

where

$$\tilde{S}_{i,j} = (\lambda_1/k) S_{i,j}. \tag{3.31}$$

In a similar way, replacing $\cos^2 v$, $\sin^2 v$ and $\sin 2v$ in (3.21) by their spline interpolants (B-spline coefficients γ_j, δ_j and ϵ_j) finally results in the condition

$$c_{-k+2,j} = S_{0,0} + (1 + \lambda_2/\lambda_1)(\alpha_j \tilde{S}_{1,0} + \beta_j \tilde{S}_{0,1}) + \gamma_j S^*_{2,0} + \delta_j S^*_{0,2} + \epsilon_j S^*_{1,1},$$
$$j = -l, \dots, h, \tag{3.32}$$

where

$$S^*_{i,j} = [\lambda_1 \lambda_2 / k(k-1)] S_{i,j}. \tag{3.33}$$

Now, if we have an odd number of knots in the v-direction such that

$$h = 2n - 1 \tag{3.34}$$

and

$$\mu_{j+n} = \mu_j + \pi, \quad j = 0, 1, \dots, n, \tag{3.35}$$

then, analogously to (3.16),

$$N_{j,l+1}(v) \equiv N_{j+n,l+1}(v + \pi), \quad j = -l, \dots, n-1. \tag{3.36}$$

Therefore, considering the properties $\cos(v + \pi) = -\cos v$, $\sin(v + \pi) = -\sin v$, the B-spline coefficients of our spline interpolants will also be such that

$$\alpha_{j+n} = -\alpha_j, \qquad \beta_{j+n} = -\beta_j, \qquad \gamma_{j+n} = \gamma_j, \qquad \delta_{j+n} = \delta_j, \qquad \epsilon_{j+n} = \epsilon_j,$$
$$j = -l, \dots, n-1. \tag{3.37}$$

So, from (3.29), (3.30), (3.36) and (3.37), we can easily derive that

$$\frac{\partial s(0, v)}{\partial u} \equiv -\frac{\partial s(0, v + \pi)}{\partial u}, \quad -\pi \leqslant v \leqslant 0, \tag{3.38}$$

and analogously also that

$$\frac{\partial^2 s(0, v)}{\partial u^2} \equiv \frac{\partial^2 s(0, v + \pi)}{\partial u^2}, \quad -\pi \leqslant v \leqslant 0. \tag{3.39}$$

We may conclude then that although $S(x, y)$ has only approximately C^2 continuity at the origin, at least this property is guaranteed for any curve $S(t \cos \omega, t \sin \omega)$, $-1 \leqslant t \leqslant 1$ (the intersection of the graph of $S(x, y)$ with any plane $x \sin \omega + y \cos \omega = 0$).

4. Smoothing data over the circle

We are ready now to consider the problem of fitting a smooth function $S(x, y)$ to data z_q (weights w_q) given at points (x_q, y_q), $q = 1, 2, \dots, m$, scattered arbitrarily over the unit disc. Through the inverse mapping of (2.1), i.e.

$$u = \sqrt{x^2 + y^2}, \quad v = \arctan(y/x), \qquad (x, y) \in C, \tag{4.1}$$

we can determine corresponding points (u_q, v_q) on the rectangle D. The problem is then reduced to finding a smooth tensor product spline on D such that $s(u_q, v_q) \approx z_q$. Let us first recall the basic principles of the general smoothing algorithm described in [4]. Then we can indicate how it must be adapted to find a smoothing spline that satisfies the additional constraints (3.19)–(3.21). In the unconstrained case, a spline $s(u, v)$ is determined as the solution of the following minimization problem:

Minimize

$$\eta(\bar{c}) = \sum_{q=1}^{g} \sum_{j=-l}^{h} \left(\sum_{i=-k}^{g} a_{i,q} c_{i,j} \right)^2 + \sum_{r=1}^{h} \sum_{i=-k}^{g} \left(\sum_{j=-l}^{h} b_{j,r} c_{i,j} \right)^2, \tag{4.2}$$

subject to the constraint

$$\sigma(\bar{c}) = \sum_{q=1}^{m} w_q \left(z_q - s(u_q, v_q) \right)^2 \leqslant S. \tag{4.3}$$

The quantity $\eta(\bar{c})$ refers to the conditions (3.11)–(3.12). Therefore, it can be seen as a measure of the (lack of) smoothness of fit. Closeness of fit is measured through $\sigma(\bar{c})$. The parameter S, which is supplied by the user, controls the extent to which these two (very often contradictory) properties are satisfied. Let us suppose for the moment that S is such that condition (4.3) is feasible. It is clear that this will depend also on the number and the position of the knots of $s(u, v)$.

In order to solve the above minimization problem, consider first the following overdetermined system of equations

$$\begin{aligned}
&\sqrt{w_q} \sum_{i=-k}^{g} \sum_{j=-l}^{h} c_{i,j} M_{i,k+1}(u_q) N_{j,l+1}(v_q) = \sqrt{w_q}\, z_q, \quad 1, 2, \ldots, m, \\
&\frac{1}{\sqrt{p}} \sum_{i=-k}^{g} a_{i,q} c_{i,j} = 0, \qquad q = 1, 2, \ldots, g, \quad j = -l, \ldots, h, \\
&\frac{1}{\sqrt{p}} \sum_{j=-l}^{h} b_{j,r} c_{i,j} = 0, \qquad r = 1, 2, \ldots, h, \quad i = -k, \ldots, g.
\end{aligned} \tag{4.4}$$

These equations will be solved in the sense of least-squares, i.e. such that $\sigma(\bar{c}) + p^{-1}\eta(\bar{c})$ is minimal, p being a parameter which dictates the trade-off between fitting and smoothing. Let $s_p(u, v)$ denote the corresponding spline.

It is then easily verified that, using the method of Lagrange, problem (4.2)–(4.3) simply results in the computation of the B-spline coefficients $\bar{c}$ from (4.4) when p is given the value of the positive root of the equation $F(p) = S$ with

$$F(p) = \sum_{q=1}^{m} w_q \left(z_q - s_p(u_q, v_q) \right)^2. \tag{4.5}$$

The smoothing spline $s_p(u, v)$ has the following properties [4]:

(i) To each positive p there corresponds a single spline $s_p(u, v)$, the B-spline coefficients of which are the (minimal-length) solution of (4.4).

(ii) As p tends to infinity, $s_p(u, v)$ becomes the least-squares spline $S_{g,h}(u, v)$.

(iii) As p tends to zero, $s_p(u, v)$ becomes the least-squares polynomial $P_{k,l}(u, v)$ of degree k in u and l in v.

(iv) $F(p)$ is a continuous, strictly decreasing and convex function for $p > 0$.

Therefore we know that, once a set of knots is found such that

$$F_{g,h}(\infty) \leqslant S < F(0), \tag{4.6}$$

with

$$F(0) = \sum_{q=1}^{m} w_q\left(z_q - P_{k,l}(u_q, v_q)\right)^2, \tag{4.7}$$

$$F_{g,h}(\infty) = \sum_{q=1}^{m} w_q\left(z_q - S_{g,h}(u_q, v_q)\right)^2, \tag{4.8}$$

there exists a single spline $s_p(u, v)$ with these knots for which $F(p) = S$. This value of p can then be determined iteratively by means of a rational interpolation scheme [4].

To find a set of knots which satisfies (4.6) we proceed in the following manner. First we determine the least-squares polynomial $P_{k,l}(u, v)$ which simply is the least-squares spline $S_{0,0}(u, v)$. If $F_{0,0}(\infty) \leqslant S$ this polynomial is a solution of our problem. However, usually we will find that $F_{0,0}(\infty) > S$. In that case we determine successive least-squares splines $S_{g,h}(u, v)$ with an increasing number of knots. At each iteration we locate one additional knot where the fit $S_{g,h}(u, v)$ is particularly poor (for more details, see [4]). So the strategy for locating knots is adaptive in the sense that there will be more knots if S is small and fewer if it is large and also in the sense that the spline will have more knots in those regions where the function underlying the data is difficult to approximate then where it has a smooth behaviour.

Now, to obtain a function $S(x, y)$ which is sufficiently smooth on C, we will solve the problem (4.2)–(4.3) and the resulting system (4.4) subject to the additional constraints (3.18), (3.23), (3.30) and (3.32). After eliminating these constraint equations, a system is obtained in the coefficients $S_{0,0}$, $\tilde{S}_{1,0}$, $\tilde{S}_{0,1}$, $S^*_{2,0}$, $S^*_{0,2}$, $S^*_{1,1}$, $c_{i,j}$, $i = -k+3, -k+4, -k+5, \ldots, g$; $j = -l, -l+1, \ldots, h-l$. It is solved in a stable way using an orthogonalization method with Givens rotations without square roots [7]. Advantage is hereby taken from the special bandstructure (see e.g. [6] for a detailed description in a similar problem). The iterative determination of the root of $F(p) = S$, now with the constrained spline $\tilde{s}_p(u, v)$ instead of $s_p(u, v)$ in the definition (4.5) of F, can be carried out in the same way as for the general smoothing spline, since $\tilde{s}_p$ has similar properties as s_p. If p tends to zero, $\tilde{s}_p(u, v)$ will now become a least-square polynomial $\tilde{P}_{k,0}(u, v)$ still of degree k in u but of degree 0 in the variable v as follows from the periodicity property (3.17).

So, also taking account of the C^2 conditions (3.20) and (3.21) which will be satisfied exactly by this polynomial, we may just as well write that

$$\tilde{P}_{k,0}(u, v) \equiv p_k(u), \qquad 0 \leqslant u \leqslant 1, \quad -\pi \leqslant v \leqslant \pi, \tag{4.9}$$

with $p_k(u)$ a polynomial of degree k, satisfying

$$p_k'(0) = p_k''(0) = 0. \tag{4.10}$$

Also, the strategy for finding a suitable set of knots can readily be adapted. If $F(0)$, now corresponding to the least-squares polynomial $\tilde{P}_{k,0}(u, v)$, is greater than S we determine successive constrained least-squares splines $\tilde{S}_{g,h}(u, v)$ until again (4.6) is satisfied. We start this iteration process with the spline $\tilde{S}_{1,7}(u, v)$ according to the knots $\lambda_1 = 0.5$, $\mu_j = \frac{1}{4}\pi(j-4)$, $j = 1, 2, \ldots, 7$. The spline interpolants for the trigonometric functions are then already reasonable accurate (maximal absolute error ≈ 0.001 for $\cos v$ and $\sin v$, ≈ 0.01 for $\cos^2 v$ and $\sin^2 v$, ≈ 0.02 for $\sin 2v$). For the reasons explained at the end of Section 3, we also add two knots instead of one (according to (3.34)–(3.35)) every time the v-direction is chosen.

5. Generalizations

The proposed method can easily be extended. Suppose that we have an approximation domain C^* with a boundary that can be described in polar coordinates through a smooth periodic function R, i.e. if $C^* = \{(x, y) \mid x^2 + y^2 \leqslant R^2(\arctan(y/x))\}$. Instead of (2.1) we can use the following mapping

$$x = uR(v)\cos v, \quad y = uR(v)\sin v, \qquad 0 \leqslant u \leqslant 1, \quad -\pi \leqslant v \leqslant \pi, \tag{5.1}$$

and once again find a spline approximation s on D for $f(u, v) = F(x, y)$. The conditions for C^2 continuity can be derived in a similar way as described in Section 2. We obtain

$$\frac{\partial f}{\partial u}(0, v) = R(v)(F_{1,0}\cos v + F_{0,1}\sin v) \tag{5.2}$$

and

$$\frac{\partial^2 f}{\partial u^2}(0, v) = R^2(v)\left(F_{2,0}\cos^2 v + F_{0,2}\sin^2 v + F_{1,1}\sin 2v\right), \tag{5.3}$$

instead of (2.12) and (2.18). So, the smoothing algorithm of Section 4 is very easily adapted. Instead of (4.1), we simply use the mapping

$$u = \sqrt{x^2 + y^2}/R(v), \quad v = \arctan(y/x), \qquad (x, y) \in C^*, \tag{5.4}$$

to obtain the corresponding set of data points (u_q, v_q) on D. The constraints (3.18), (3.23), (3.30) and (3.32) are maintained on the understanding that the parameters α_j, β_j, γ_j, δ_j and ϵ_j must be seen now as the B-spline coefficients of the interpolants for $R(v)\cos v$, $R(v)\sin v$, $R^2(v)\cos^2 v$, $R^2(v)\sin^2 v$ and $R^2(v)\sin 2v$.

Often, the reason for choosing a non-rectangular approximation domain C^* is that we know some additional constrains for F at the boundary. Suppose for example that we are given the value of F, i.e. that we know a function Z such that

$$f(1, v) = Z(v), \quad -\pi \leqslant v \leqslant \pi. \tag{5.5}$$

How can we then implement such a constraint into our spline approximation? If we choose the boundary knots $\lambda_{g+2} = \lambda_{g+3} = \cdots = \lambda_{g+k+1} = 1$ then

$$M_{i,k+1}(1) = \delta_{i,g}, \tag{5.6}$$

and consequently from (3.5),

$$s(1, v) = \sum_{j=-l}^{h} c_{g,j} N_{j,l+1}(v). \tag{5.7}$$

So, if Z is identically zero, (5.5) simply results in

$$c_{g,j} = 0, \quad j = -l, \ldots, h. \tag{5.8}$$

This additional condition for the B-spline coefficients can then very easily be implemented into our approximation algorithm. If Z has a constant value Z^*, we can first calculate new function values $z_q^* = z_q - Z^*$ and determine a corresponding spline $s^*(u, v)$ with B-spline coefficients $c_{i,j}^*$ satisfying the constraints (3.18), (3.23), (3.30), (3.32) and (5.8). The requested spline $s(u, v)$ will have then coefficients $c_{i,j} = c_{i,j}^* + Z^*$ as follows from property (3.8). Finally, if Z is an arbitrary periodic function with a continuous second derivative, we can proceed as follows. Instead of $f(u, v)$ we will approximate

$$\tilde{f}(u, v) = f(u, v) - u^3 Z(v). \tag{5.9}$$

This function also satisfies the conditions (2.2), (5.2) and (5.3), and moreover,

$$\tilde{f}(1, v) \equiv 0. \tag{5.10}$$

So, starting from the function values $\tilde{z}_q = z_q - u_q^3 Z(v_q)$ we will determine a spline $\tilde{s}(u, v)$ in the same way as for $s(u, v)$. If $\tilde{S}(x, y)$ denotes the corresponding function on C^*, then $F(x, y)$ is finally approximated by

$$S(x, y) = \tilde{S}(x, y) + (x^2 + y^2)^{3/2} Z(v)/R^3(v), \tag{5.11}$$

with v given by (5.4).

6. Practical considerations and examples

The algorithm described in Sections 4 and 5 has been implemented in a Fortran subroutine package, called SMOCIR. A copy of this package together with an example program can be obtained from the author, on magnetic tape.

Apart from the set of data points (x_q, y_q, z_q) with the corresponding weights w_q, $q = 1, 2, \ldots, m$, the user must specify the approximation domain C^* through a periodic function R and provide the smoothing factor S to control the trade-off between closeness of fit and smoothness of fit. Recommended values for S depend on the weights w_q. If available, one should use an estimate δ_q of the standard deviation of the error in z_q and set $w_q = (\delta_q)^{-2}$. If this value is used for w_q, then a good S-value should be found in the range $m \pm \sqrt{2m}$ [8]. More practical considerations as concerned the choice of S can be found in [4].

The program returns a bicubic ($k = l = 3$) spline approximation $s(u, v)$ on $D = [0, 1] \times [-\pi, \pi]$ with automatically located knots. The requested approximation $S(x, y) = s(u, v)$ on C^* can then be found through formula (5.4).

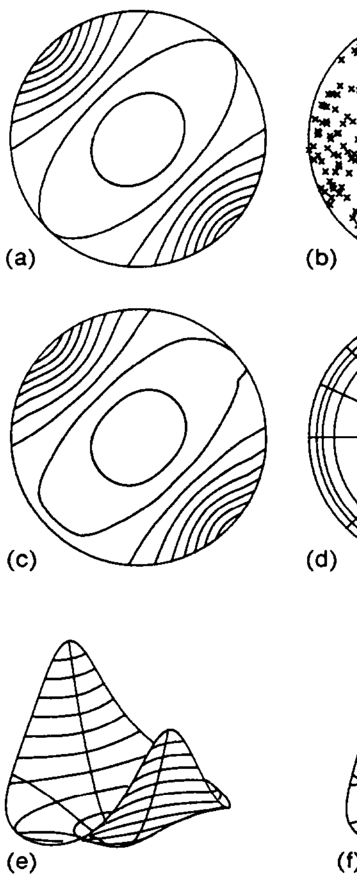
We now give some examples of approximations constructed by means of SMOCIR.

Example 1. Using a random number generator we generated

- a set of 400 points (x_q, y_q), scattered uniformly over the unit disc ($R(v) \equiv 1$).
- a set of normally distributed stochastic variates e_q, with expected value (EV) 0 and standard deviation (SD) 0.01.

Then we considered the data (x_q, y_q), $z_q = F(x_q, y_q) + e_q$, $w_q = (0.01)^{-2}$, $q = 1, 2, \ldots, 400$ in order to find an approximation $S(x, y)$ for $F(x, y) = (x^2 + y^2)/((x + y)^2 + 0.5)$.

In Fig. 1 we give some results. Fig. 1(a) shows a contour map of $F(x, y)$ (function values



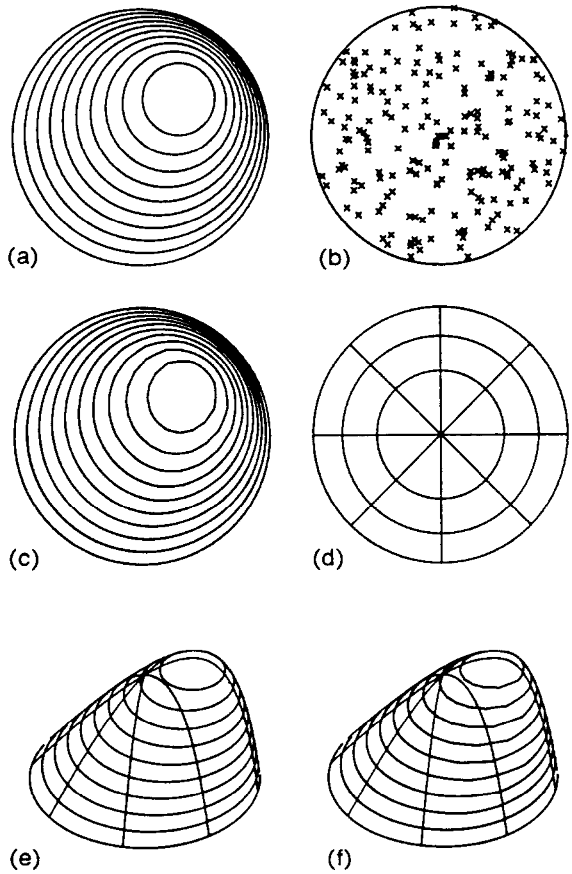


Fig. 1. Spline approximation $S(x, y)$ for $F(x, y) = (x^2 + y^2)/((x + y)^2 + 0.5)$ on the unit disc. (a) Contour map of $F(x, y)$, (b) Position of the data points, (c) Contour map of $S(x, y)$, (d) Knot distribution, (e) Perspective view of $F(x, y)$, (f) Perspective view of $S(x, y)$.

Fig. 2. Spline approximation $S(x, y)$ for $F(x, y) = 1 - [(3x - 1)^2 + (3y - 1)^2][11 - 6x - 6y]^{-1}$ on the unit disc. (a) Contour map of $F(x, y)$, (b) Position of the data points, (c) Contour map of $S(x, y)$, (d) Knot distribution, (e) Perspective view of $F(x, y)$, (f) Perspective view of $S(x, y)$.

0.2, 0.4, ..., 1.8). In Fig. 1(b) we have marked the position of the different data points (x_q, y_q). The contour map of Fig. 1(c) corresponds to an approximation $S(x, y)$ with smoothing factor $S = 400$. The corresponding tensor spline $s(u, v)$ on the rectangle D has $g = 4$ knots in the u-direction and $h = 11$ knots in the v-direction. While D is further subdivided into rectangular panels $D_{i,j}$ by the intersection of knots, a non-rectangular geometry of panels is obtained after transformation to the circle, as can be seen in Fig. 1(d). A such-like geometry of panels could in fact be a reason in itself for choosing a non-rectangular approximation domain, for example to cope more efficiently with radially changing difficulties in F. Finally in Fig. 1(e) and 1(f) we see a three-dimensional depiction of $F(x, y)$ and its approximation. The quality of fit of $S(x, y)$ may certainly be judged satisfactory although it seems somewhat inferior towards the boundary.

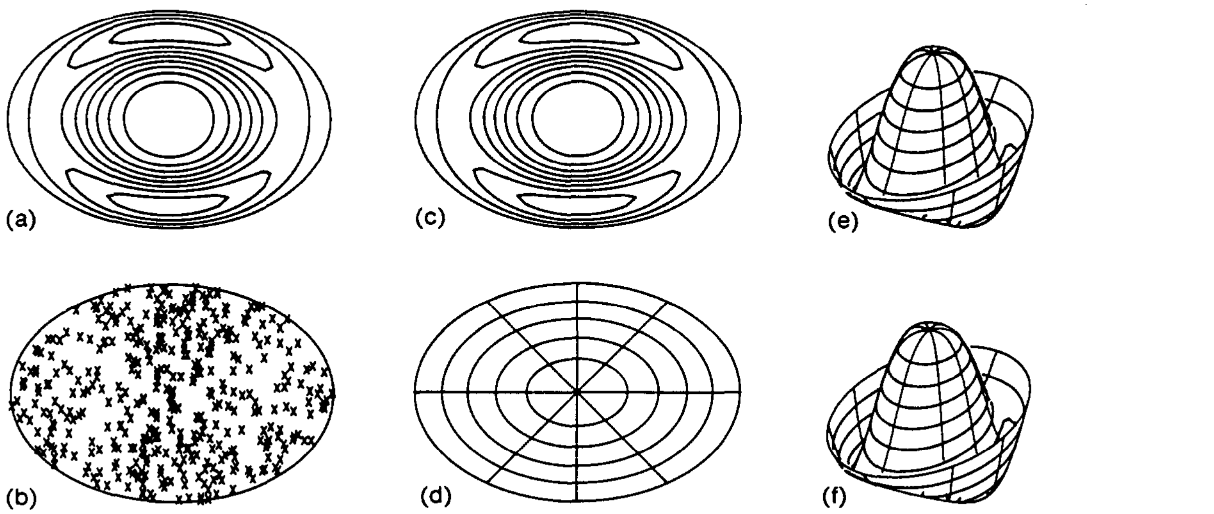


Fig. 3. Spline approximation $S(x, y)$ for $F(x, y) = \exp(-2x^2 - y^2)\cos(3\pi(4x^2 + 9y^2)/8)$ over the ellipse $4x^2 + 9y^2 \leqslant 4$. (a) Contour map of $F(x, y)$, (b) Position of the data points, (c) Contour map of $S(x, y)$, (d) Knot distribution. (e) Perspective view of $F(x, y)$, (f) Perspective view of $S(x, y)$.

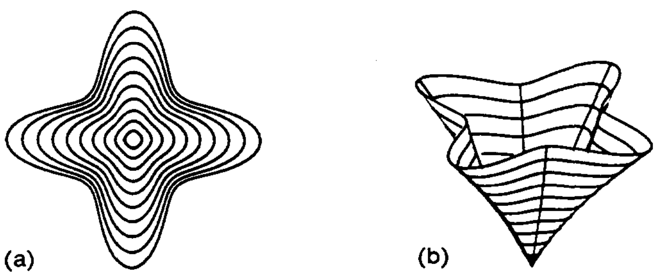


Fig. 4. Spline approximation $S(x, y)$ for $F(x, y) = \mathrm{tg}\{\pi(x^2 + y^2)^2(2(x^2 - y^2)^2 + 3(x^2 + y^2)^{3/2})^{-1}\}$ (a) Contour map of $S(x, y)$, (b) Perspective view of $S(x, y)$.

Example 2. The quality of fit can still be improved if we can impose additional boundary conditions. The program SMOCIR offers the possibility to determine a function $S(x, y)$ which becomes identically zero at the boundary. In a second example, we therefore considered the approximation of a function $F(x, y) = 1 - ((3x - 1)^2 + (3y - 1)^2)/(11 - 6x - 6y)$, again on the unit disc C. In a similar way as for the first example, we generated a set of data, now only 192 points and with larger stochastic errors (EV = 0, SD = 0.02). Fig. 2 shows the approximation results for a function $S(x, y)$ corresponding to a smoothing factor $S = 200$ (all $w_q = (0.02)^{-2}$). The quality of fit is very good now. Fig. 2(f) also shows that $S(x, y)$ is indeed sufficiently smooth at the origin.

Example 3. In a third example, we considered the approximation of $F(x, y) = \exp(-2x^2 - y^2)\cos(3\pi(4x^2 + 9y^2)/8)$ on the ellipse $4x^2 + 9y^2 \leqslant 4$. The boundary of this domain is described in polar coordinates through the function $R(v) = 2\ (9 - 5\cos^2 v)^{-1/2}$. We generated 400 data points with stochastic errors of about 1% (SD = 0.01). Figure 3 shows the approximation results for a function $S(x,y)$ vanishing at the boundary at the boundary and corresponding to a smoothing factor $S = 400$ (all $w_q = (0.01)^{-2}$). The graphs for $F(x,y)$ and $S(x,y)$ are hardly distinguishable.

Example 4. The package SMOCIR offers even more possibilities. The user can select the requested order of continuity at the origin (C^0, C^1 or C^2) and he can also obtain a tensor spline $s(u,v)$ in the least-squares sense if he provides the knots λ_i and μ_j. These two options were used to find a function $S(x,y)$ of only C^0 continuity at the origin and interpolating $F(x,y) = \mathrm{tg}(\pi(x^2+y^2)^2/(2(x^2-y^2)^2+3(x^2+y^2)^{3/2})$ at 145 points. The results are shown in Fig. 4. The approximation domain corresponds to the function $R(v) = 3(3-\cos 4v)^{-1}$.

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