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AN OPTIMAL BICUBIC SPLINE ON A RECTILINEAR MESH OVER A RECTANGLE

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ABSTRACT

For a function of two variables, we construct an optimal bicubic spline which interpolates to specified function values at the grid-points of a rectilinear mesh over a rectangle. Additional conditions in the form of normal derivatives may be specified. By optimality, we mean that third derivative discontinuities are minimized in the least square sense.

INTRODUCTION

The Domain and Mesh

We consider a closed rectangular domain

$$R \equiv I_x \times I_y$$

where

$$I_x \equiv [\underline{x}, \overline{x}] \quad \text{with } \overline{x} > \underline{x}$$

$$I_y \equiv [\underline{y}, \overline{y}] \quad \text{with } \overline{y} > \underline{y}.$$

We further consider a partition of I_x by points $\underline{x} = x_1, x_2, \ldots, x_m = \overline{x}$ with $m \geq 5$ and a partition of I_y by $\underline{y}=y_1, y_2, \ldots y_n$ with $n \geq 5$. Neither partition need be uniform, but the points x_i for i=1 to m and y_j for j=1 to n must be strictly increasing with i and j respectively.

We call the mn points (x_i, y_j) for i=1 to m and j=1 to n grid-points for the mesh over R. See Figure 1.

The Bicubic Spline

As given in 1, the bicubic spline, u(x,y), defined on R with knots at the grid-points, (x_i, y_j) for i=1 to m and j=1 to n has the following properties:

1. On any subrectangle, $[x_i, x_{i+1}] \times [y_i, y_{i+1}]$, u is a bicubic polynomial in x and y; i.e.,

$$u(x, y) = \sum_{\ell=0}^{3} \sum_{k=0}^{3} \alpha_{\ell k} x^{\ell} y^{k}$$

2. The bicubic spline has continuous second derivatives on R; i.e., u_{xx}, u_{xy} and u_{yy} are continuous on R.

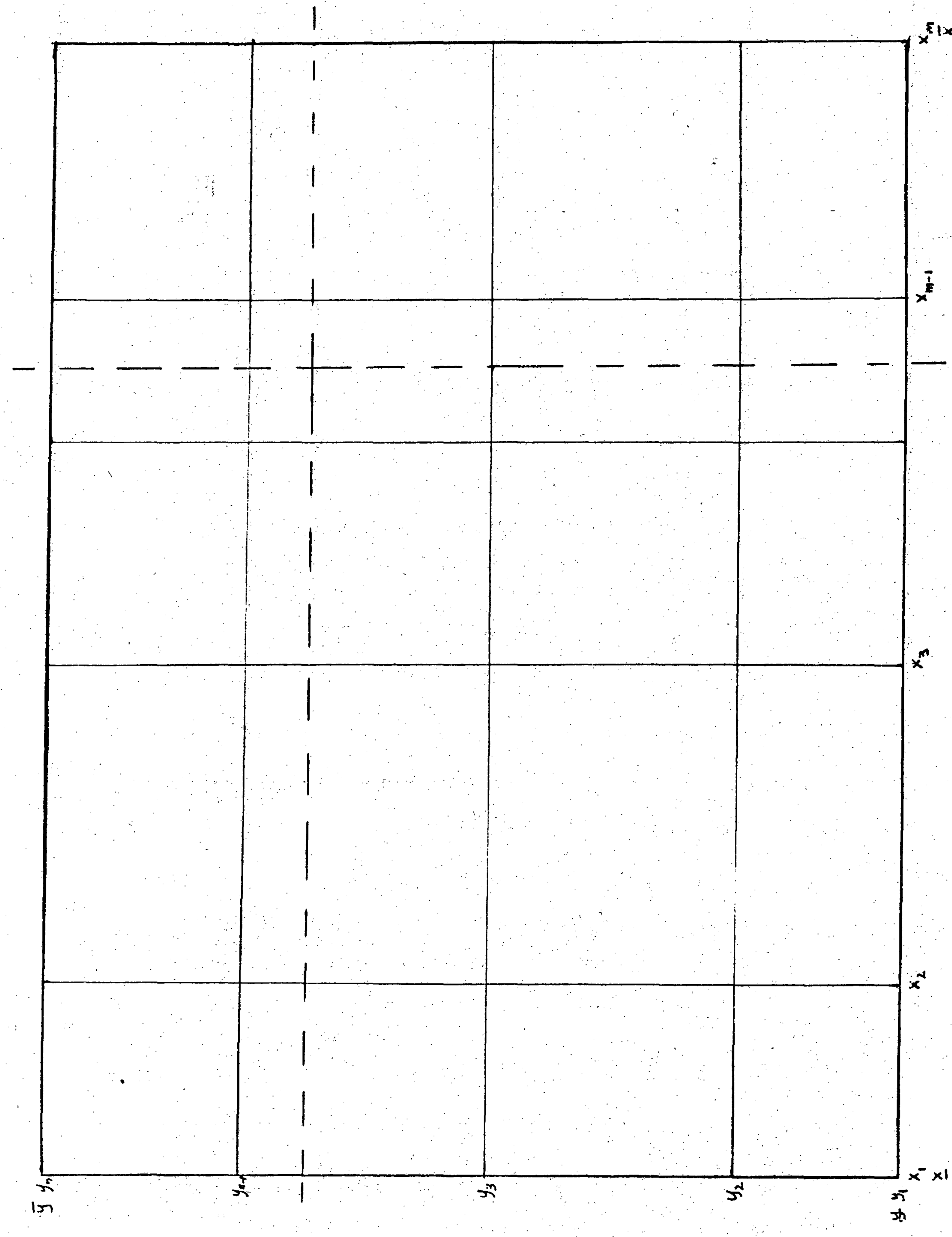

FIGURE 1

The following properties are readily deduced[1]

3. For any fixed $y=y_*$ (in particular for any grid-line $y=y_j$) the functions, $u(x,y_*)$ <u>and</u> $u_y(x, y_*)$ are cubic splines in x.

4. For any fixed $x=x_*$ (in particular for any grid-line $x=x_i$) the functions, $u(x_*,y)$ and $u_x(x_*,y)$ are cubic splines in y.

5. On any subrectangle the bicubic polynomial "segment" of u is uniquely determined when u, u_x, u_y and u_{xy} are known at each of its four vertices. (The sixteen values specified determine the sixteen coefficients $\alpha_{\ell k}$).

6. On the retangle, R, the bicubic spline, u, is uniquely determined when u is known at all grid-points, when the normal derivative u_x, is known the boundary grid-points, (x_1, y_j) and (x_m, y_j) and u_y is known at the points, (x_i, y_1) and (x_i, y_n) and the cross-derivative u_{xy} is known at the four grid-points (vertices of R) (x_1, y_1), (x_m, y_1), (x_m, y_n) and (x_1, y_n). (A cubic spline is uniquely determined when its values at its knots and its terminal first derivatives are known, consequently the values required by property 5 can be readily computed by virtue of properties 3 and 4.)

Optimization

From property 6 above, we see that the bicubic spline on R with knots (x_i, y_j) for i=1 to m and j=1 to n is uniquely determined by mn + 2m + 2n + 4 parameters, namely

(a) The mn values of u at the grid-points

(b) The 2m values of u_y at grid-points along y_1 and y_n

(c) The 2n values of u_x at grid-points along x_1 and x_m

(d) The 4 values of u_{xy} at the corners.

If all these parameters are in fact specified, then the bicubic spline u is determined exactly and no optimization is possible. In general u, u_x and u_y will have third derivative discontinuities at the internal grid-points.

If we assume that the mn parameters (a) are always specified but that some or all of the remaining parameter sets are not, then we are free to compute values for the unspecified parameters which will minimize in the least square sense the afore-mentioned third-derivative discontinuities. The "smoothest" bicubic spline thus obtained is called the optimal bicubic spline for the given conditions. In the succeeding section we consider the construction of this bicubic spline under a reasonable variety of circumstances.

CONSTRUCTION OF THE OPTIMAL BICUBIC SPLINE

In general the construction of an optimal cubic spline involves the following

(a) Prescription

(b) Specification

(c) Optimization

(d) Evaluation

In (a) we prescribe the knots. This is done adequately by providing values for x_i for i=1 to m and y_j for j=1 to n. In general we must have $m \geq 5$ and $n \geq 5$. The sets $\{x_i\}$ and $\{y_j\}$ must be strictly increasing with respect to the pertinent index. Spacing need not be uniform.

In (b) we specify known values relative to u. We must always provide all values

$$u_{ij} = u(x_i, y_j) \text{ for } i=1 \text{ to } m \text{ and } j=1 \text{ to } n$$

and none or any or all of the following sets of values:

(1) $u_y(x_i, y_1)$ for i=1 to m

(2) $u_x(x_m, y_j)$ for j=1 to n

(3) $u_y(x_i, y_n)$ for i=1 to m

(4) $u_x(x_1, y_j)$ for j=1 to n

In case all the boundary normal-derivatives are specified, we may also specify the cross derivatives

$$u_{xy}(x_1, y_1) \text{ , } u_{xy}(x_m, y_1) \text{ , } u_{xy}(x_m, y_n) \text{ and } u_{xy}(x_1, y_n)$$

For this case no optimization is possible and we proceed to evaluation.

In (c) we compute values not specified above for boundary normal derivatives and corner cross-derivatives. These computed values are optimal in that they minimize third derivative discontinuities in the least square sense.

In (d) we compute values for u_x, u_y and u_{xy} (not otherwise specifed or computed) at every grid-point, (x_i, y_j). From these values (in accordance with property 6) values for u and any desired first or second derivatives may be computed at any point (x, y) in any subrectangle and, consequently at any point in R.

OPTIMIZATION

In the simplest case for optimization, we know u at all grid-points and all normal derivatives at boundary grid-points.

Let $s_i = u_y(x_i, y_1)$ for i=1 to m and from the point set, (x_i, s_i) for i=1 to m determine[2] the optimal values for $s''(x_1)$ and $s''(x_m)$ so that the cubic spline s has minimum third derivative discontinuity and compute $s'(x_1)$ and $s'(x_m)$. We then set

$$u_{xy}(x_1, y_1) = s'(x_1)$$

and $$u_{xy}(x_m, y_1) = s'(x_m)$$

In effect we have minimized the discontinuity in u_{yxxx} along y_1.

Similarly, let $t_i = u_y(x_i, y_n)$ compute the optimal cubic spline t and obtain, $t'(x_1)$ and $t'(m)$ and then set

$$u_{xy}(x_1, y_n) = t'(x_1)$$

$$u_{xy}(x_m, y_n) = t'(x_m)$$

In effect we have minimized the discontinuity in u_{yxxx} along y_n.

We can apply the same process to $u_x(x_1, y_j)$ and $u_x(x_m, y_j)$ obtain values for

$$u_{xy}(x_1, y_1) \text{ and } u_{xy}(x_1, y_n)$$

and $$u_{xy}(x_m, y_1) \text{ and } u_{xy}(x_m, y_n)$$

Essentially we have minimized the discontinuity in u_{xyyy} along x_1 and x_m.

Now it is unlikely that corresponding corner values for u_{yx} and u_{xy} will be in full agreement. We believe that with most data the disagreement will not be great and a reasonable modicum of optimality can be attained by using the averages of corresponding u_{yx} and u_{xy} for optimal corner values of the cross-derivative.

If the above method does not seem satisfactory for some data, a procedure can be readily devised for minimizing simultaneously the third derivative discontinuities in all four boundary normal derivative cubic splines subject to four parameters, namely, the values of u_{xy} at the four corners.

In the next case of optimization we consider that we know u at all grid-points and u_y at grid-points along boundaries $y=y_m$, and $y=y_n$. To find u_x at grid-points along $x=x_1$ and $x=x_m$, we set for j=1 to n

$$r_j(x_i) = u_{ij}$$

and solve for the optimal cubic splines $r_j(x)$ and set

$$u_x(x_1, y_j) = r_j'(x_1)$$

$$u_x(x_m, y_j) = r_j'(x_m)$$

In effect we have minimized the discontinuity of u_{xxx}, We now proceed as in the simplest case.

The case where we know u at all grid-points and u_x at grid-points along x_1 and x_m is treated in an analogus manner.

We now consider the case where u is known at all grid-points and u_x is known only at grid-points along $x=x_1$. In this case we must first solve for optimizing values for u_x at grid-points along $x=x_m$. We set for j=1 to n

$$r_j(x_i) = u_{ij}$$

and

$$r_j(x_1) = u_x(x_1, y_j)$$

Then we use a one-parameter (the value of $r''(x_m)$) to determine an optimal cubic spline, $r_j(x)$ for which third derivative discontinuities are minimized. Again we are minimizing discontinuities in u_{xxx}. We now set

$$u_x(x_m, y_j) = r_j'(x_m)$$

and proceed as outlined above.

When only u_x is known along x_m, or u_y along y_1 or u_y along y_n, the procedure is analogous to that just described. Likewise any combination of specifications of boundary normal derivative sets can be handled.

The most complete case for optimization occurs when only values for u are known at the grid-points. In this case we compute optimal cubic splines in x for $u(x_i, y_j)$ for every j and in y for $u(x_i, y_j)$ for every i thereby determining optimizing values for normal derivatives at all boundary grid-points. We then proceed as in the first paragraph of this section. It is interesting to note that in this case alternative values u_{yx} and u_{xy} at the corners do agree.

EVALUATION

After the optimization process (if any) we need to compute values for u_x, u_y and u_{xy} at all grid-points where they are not presently known.

We set for j=1, n

$$r_{ji} = u_{ij}$$

$$r'_{j1} = u_1(x_1, y_j)$$

$$r'_{jm} = u(x_m, y_j)$$

and for the (uniquely determined) cubic spline $r_j(x)$ we compute

$$r'_j(x_i) \text{ for } i=2 \text{ to } m-1$$

and set

$$u_x(x_i, y_j) = r'_j(x_i).$$

By a similar process for i=1 to m we obtain

$$u_y(x_i, y_j) \text{ for } j=2 \text{ to } n-1.$$

For j=1 and n, we use the corresponding cubic spline in x for u_y with the known values of u_{xy} as terminal derivatives to compute

$$\left.\begin{array}{l} u_{xy}(x_i, y_1) \\ \\ u_{xy}(x_x, y_n) \end{array}\right\} \text{ for } i = 2 \text{ to } m-1.$$

and

For i=1 to m, we use cubic splines in y corresponding to $u_x(x_i, y_j)$ having terminal first derivatives $u_{xy}(x_i, y_1)$ and $u_{xy}(x_i, y_n)$ to determine

$$u_{xy}(x_i, y_j) \text{ for } j=2 \text{ to } n-1.$$

COMPUTER CODE

A FORTRAN computer subroutine, OBCSPY, has been written to perform the computation described in the optimization and evaluation sections above. Under its various options, any of the specifications discussed above and, as well, the case where the bicubic spline is completely specified can be handled by the code. Listings and instructions for use of OBCSPY can be obtained from the authors.

CONCLUSION

The problem of surface fitting over a rectangle for a function, $f(x, y)$, when f is known only at grid-points of a rectilinear mesh over and including the boundaries of R is readily handled by the technique described above. We simply set $u_{ij} = f(x_i, y_j)$ and compute the optimal bicubic spline u. Cases where boundary normal derivatives for f are known can likewise be solved by simply requiring u to agree with f in these particulars.

Like cubic spline fitting[3], bicubic spline fitting has the advantage over local (relatively low degee) bipolynomial fitting in that it obtains second derivative continuity over all of R. Its advantage over high degree bipolynomial fitting is that it avoids the extreme inflection which sometimes occurs under the latter. In contrast with least square bipolynomial fitting the bicubic spline is an exact fit of known data while the latter is not.

Bicubic spline fitting is quite convenient for interpolation to obtain approximated values of the fitted function f at any non-grid point in R. Let (x^*, y^*) be such a point, then (x^*, y^*) lies in the interior of some sub-rectangle $(x_i, x_{i+1}) \times (y_j, y_{j+1})$. We compute $u(x^*, y^*)$ as an approximation for $f(x^*, y^*)$. We use the fact that u and u_y are cubic in x between x_i and x_{i+1} along both y_j and y_{j+1}. The known values of u, u_y and u_{xy} at (x_i, y_j) and (x_{i+1}, y_j) are sufficient to determine u and u_y at (x^*, y_j). Similarly we can determine u and u_y at (x^*, y_{j+1}). We use the fact that u is a cubic in y between y_j and y_{j+1} along x^*, and the values for u an u_y at (x^*, y_j) and (x^*, y_{j+1}) sufficient to determine $u(x^*, y^*)$.

ACKNOWLEDGEMENT

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