ON FITTING A SURFACE

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This article deals with the problem of fitting the surface $f=g(x)\,h(y)$ to the set of points $(x_i, y_j, f_{i,j})$. Functions $g(x)$ and $h(y)$ are supposed to be expressible in terms of orthonormal sets of functions. The desired coefficients of these functions are determined as characteristic vectors corresponding to the largest characteristic root of two matrices having common characteristic roots.

FORMULATION OF THE PROBLEM AND ITS SOLUTION

Let the $M\,N$ points to be fitted to the surface

$$f=f\,(x, y)$$

be given by $(x_i, y_j, f_{i,j})$, $1 \leqslant i \leqslant M$, $1 \leqslant j \leqslant N$.

For the sake of simplicity, we suppose that

$$f\,(x, y) = g\,(x)\,h\,(y),$$

so that the method of least-mean-square-error gives

$$E = \sum_{i,j} [f_{i,j} - g\,(x_i)\,h\,(y_j)]^2 = \text{min.} \tag{1*}$$

Let us suppose that

$$\left.\begin{aligned} g\,(x) &= \sum_p a_p\, g_p\,(x) \\ h\,(y) &= \sum_p b_p\, h_p\,(y) \end{aligned}\right\} \tag{2**}$$

where $g_p\,(x)$ and $h_p\,(y)$, $0 \leqslant p \leqslant L$, are two orthonormal sets of functions on $(x_1, x_2, \ldots\ldots, x_M)$ and $(y_1, y_2, \ldots, y_N)$ respectively, *i.e.*,

$$\sum_i g_q(x_i)\; g_q\,(x_i) = \delta_{p,q} = \sum_j h_p\,(y_j)\; h_q\,(y_j) \tag{3}$$

$\delta_{p,q}$ denoting the Kronecker delta. From (2) and (3) we have

$$\left.\begin{aligned} \sum_i g\,(x_i)\, g_q\,(x_i) &= a_p \\ \sum_j h\,(y_j)\, h_p\,(y_j) &= b_p \end{aligned}\right\} \tag{4}$$

and, therefore, from (2) we have

$$\begin{aligned} \sum_i g^2\,(x_i) &= \sum_i \sum_{p,q} a_p\, a_q\, g_p\,(x_i)\, g_q\,(x_i) \\ &= \sum_{p,q} a_p\, a_q \sum_i g_p\,(x_i)\, g_q\,(x_i) \\ &= \sum_p a_p{}^2, \text{ from (3).} \end{aligned} \tag{5}$$

*For the simplicity of notation we fix the range of each of the summation indices; i will vary from 1 to M, j from 1 to N and p, q, r, t from 0 to L.

**The reason for taking equal number of terms in the expansions of $g\,(x)$ and $h\,(y)$ is explained in the appendix.

Similarly

$$\sum_j h^2(y_j) = \sum_p b_p^2 \ . \tag{6}$$

Making use of (2) in (1) and differentiating E with respect to b_p and with respect to a_p we have respectively

$$\left.\begin{aligned} \sum_{i,j} f_{i,j}\, g(x_i)\, h_q(y_j) &= \sum_{i,j} g^2(x_i)\, h(y_j)\, h_q(y_j) \\ \sum_{i,j} f_{i,j}\, g_p(x_i)\, h(y_j) &= \sum_{i,j} h^2(y_j)\, g(x_i)\, g_p(x_i) \end{aligned}\right\} \tag{7}$$

Using (3) in the L.H.S. and (4), (5) in the R.H.S. of above we have

$$\sum_q s_{p,q}\, b_q = B\, a_p, \quad \text{for all } p,\ 0 < p < L \tag{8}$$

$$\sum_p s_{p,q}\, a_p = A\, b_q, \quad \text{for all } q,\ 0 < q < L \tag{9}$$

where for all $p, q,\ 0 < p, q < L$

$$s_{p,q} = \sum_{i,j} f_{i,j}\, g_p(x_i)\, h_q(y_j) \tag{10}$$

and where

$$A = \sum_p a_p^2, \quad B = \sum_p b_p^2. \tag{11}$$

For the sake of simplicity, we introduce the following matrix notation

$$a = [a_0, a_1, \ldots, a_L] \tag{12}$$

$$b = [b_0, b_1, \ldots, b_L] \tag{13}$$

$$G = [g_p(x_i)],\ 0 < p < L,\ 1 < i < M \tag{14}$$

$$H = [h_q(y_j)],\ 0 < q < L,\ 1 < j < N \tag{15}$$

$$F = [f_{i,j}],\ 1 < i < M,\ 1 < j < N \tag{16}$$

$$S = [s_{p,q}],\ 0 < p, q < L \tag{17}$$

so that (8), (9) and (10) can be rewritten respectively as

$$S\, b^T = B\, a^T \tag{18}$$

$$S^T a^T = A\, b^T \tag{19}$$

$$S = G\, F\, H^T \tag{20}$$

where T stands for 'the transpose of'. Substituting from (19) into (18) and from (18) into (19) we have respectively

$$(X - \lambda)\, a^T = 0 \tag{21}$$

$$(Y - \lambda)\, b^T = 0 \tag{22}$$

where

$$X = S\, S^T, \quad Y = S^T S \tag{23}$$

and

$$\lambda = A\,B \tag{24}$$

As in curve fitting in two dimensional space, the choice of the functions $g_p(x)$ and $h_q(y)$ here also has to be made before the foregoing analysis can be applied. In other words $g_p(x_i)$ and $h_q(y_j)$ have to be supposed to be given, so that from (10) and (17), we see that S is a matrix of known elements. Thus from (21), (22) and (23) we see that the present problem reduces to the problem of determining the characteristic roots and the corresponding characteristic vectors of the matrices X and Y. It may be noted that for any two square matrices C and D, the characteristic roots of CD and DC are identical. Hence the characteristic roots of either X or Y need to be determined.

In order to determine a and b giving the minimum value of E, we first note from (1) and (2) that we can write

$$E = \sum_{i,j} f^2_{i,j} + \sum_{i,j} g^2(x_i)\,h^2(y_j) + \sum_{i,j} \sum_{p,q} {}_{i,j}\, a_p\, b_q\, g_p(x_i)\, h_q(y_j).$$

Using (5), (6), (11) in the second term and (10) in the third term above we have

$$E = \sum_{i,j} f^2_{i,j} + AB + \sum_{p,q} s_{p,q}\, a_p\, b_q \tag{25}$$

$$= \sum_{i,j} f^2_{i,j} - \lambda\,,$$

from (8) or (9) and (11), (24). (26)

The fact that X and Y are symmetric matrices makes it clear that all their characteristic roots are real. Further from (23) we see that the determinant of every principal minor of X and of Y is a positive number. In other words X and Y are matrices of positive definite form and, therefore, the characteristic roots of X and Y are non-negative (See Ferrar[1]), i.e.,

$$\lambda \geqslant 0. \tag{27}$$

From (21), (22) and (26) we see that the minimum value of E is given by λ_{max}, the greatest of the characteristic roots. A characteristic root of X and a characteristic root of Y corresponding to λ_{max} satisfying the condition

$$\sum_i a_i^2 \sum_j b_j^2 = \lambda_{max} \tag{28}$$

gives the desired product of the polynomials $g(x)$ and $h(y)$.

From the foregoing we see that the solution of the problem involves computation of the matrix products $S = GFH^T$, $X = SS^T$, $Y - S^TS$, followed by the evaluation of the characteristic roots of X or Y. The determination of the characteristic vectors corresponding to the largest of the characteristic root satisfying (28) gives the final result. Computer programs are available for making these computations and as such the numerical solution of the problem can be obtained easily.

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APPENDIX

Let the number of terms in the expansions of $g(x)$ and $h(y)$ be supposed to be L and L' respectively, such that

$$L \neq L', \tag{A1}$$

so that G and H are respectively $(L+1)\times M$ and $N\times(L''+1)$ matrices and, therefore, from (14), (15), (16) and (20) S and S^T are $(L''+1)\times(L'+1)$ and $(L'+1)\times(L+1)$ matrices respectively. Hence from (23) we see that the order of the matrix X is $(L+1)$ and that of Y is $(L'+1)$. For the sake of definiteness let

$$L' > L \tag{A2}$$

Now let S^T and S be augumented respectively by $L' - L$ columns and $L' - L$ rows all consisting of zero elements. Let these augmented matrices be denoted respectively by $S^T{}_a$ and S_a, so that $(L' + 1)$ — order matrices $S^T{}_a\, S_a$ and $S_a\, S^T{}_a$ can be written as

$$S^T{}_a\, S_a = S^T S = Y \tag{A3}$$

$$S_a\, S^T{}_a = \begin{bmatrix} S\, S^T & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} X & 0 \\ 0 & 0 \end{bmatrix} \tag{A4}$$

where zeros in (A4) denote zero matrices of appropriate order. Since $S_a S^T{}_a$ and $S^T{}_a S_a$ have the same set of characteristic roots, we see from (A3) and (A4) that while X and Y have $L + 1$ common roots, $L' - L$ additional roots of Y are all zero. From (26) we see that these roots correspond to the trivial case of the maximum value of the error given by

$$E = f^2{}_{i,j} \tag{A5}$$

and consequently from (1) and (2) we see these roots give

$$a = 0 \quad \text{or/and} \qquad b = 0 \tag{A6}$$

Obviously (A6) correspond to the trivial solution of the problem. Hence (A1) and, therefore, (A2) are meaningless assumptions, i.e.

$$L' = L$$