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PRELIMINARY DATA PROCESSING FOR A SPECIAL CLASS OF RECOGNITION PROBLEMS†

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Preliminary data processing for recognition problems in which the values of one of the indices are separable functions of two variables, given on a rectangular mesh, is considered. Algorithms by means of which structural descriptions of these functions, satisfying uniqueness and stability conditions with respect to errors of the initial data, can be found are constructed.

Modern methods of recognition and classification [1, 2] enable arbitrary sets of admissible values of the indices to be used, including those assigned by a generalized inductive definition. In order to assign a set in that way, it is necessary to indicate initial (underived) elements of that set together with a set of operations by means of which new elements can be generated. In that case, it is convenient to represent admissible values of an index in the form of structural descriptions which consist of descriptions of the individual underived elements and of the order in which the operations on them are performed. As a rule this approach, which is based on the explicit representation of structural information, enables an efficient calculation of proximity estimates to be carried out and allows economic use of the memory for storing the values of the indices. In practice, however, there is a different way of assigning values, and preliminary processing must be undertaken before structural descriptions can be obtained.

In this paper we consider the special case where the set of underived values of an index is a special family of functions of two variables, and the set of operations consists of addition only. The admissible index values and the functions of two variables at the nodes of a rectangular grid are assigned, with errors. The preliminary processing problem is to obtain a structural description of the assigned grid function.

The natural condition imposed on the required description that it shall exist and be unique imposes certain restrictions on the set of underived elements. In particular, it is possible to guarantee uniqueness by making use of additional information to narrow down the original family of functions. There is an equally natural requirement that the description should be stable with respect to errors of the initial data. In any given case small errors should not cause a change in the number of underived elements in the description.

1. CONSTRUCTING THE INITIAL SET OF DESCRIPTIONS

By an underived surface we will mean any function of two variables of the form $f(x)\,g(y)$, where $f(x)$ and $g(y)$ are arbitrary functions defined on sets $\Omega_x \subset \mathbb{R}$ and $\Omega_y \subset \mathbb{R}$, respectively, and by an

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admissible surface, any function of two variables which can be represented as the sum of a finite number of underived surfaces.

Consider the following problem. Suppose that the admissible surface

$$z(x, y) = \sum_{s=1}^{k} f_s(x)\, g_s(y) \tag{1.1}$$

is assigned with errors at the nodes of the rectangular grid (ξ_i, η_j), $\xi_i \in \Omega_x$, $\eta_j \in \Omega_y$, $i = 1, 2, \ldots, n$, $j = 1, 2, \ldots, m$, and, to fix our ideas, let $n \leq m$. The number of underived surfaces k is unknown. It is required to find a structural description of the admissible surface or in this case, to determine k and find the values of the functions $f_s(x)$, $g_s(y)$ at grid nodes.

Let M_{nm} denote the space of real $n \times m$ matrices. We introduce the matrices

$$X = [f_s(\xi_i)] \in M_{nk}, \quad Y = [g_s(\eta_j)] \in M_{mk}, \quad Z = [z(\xi_i, \eta_j)] \in M_{nm}.$$

Writing relation (1.1) at grid nodes, we obtain the matrix equation

$$XY^{\mathrm{T}} = Z \tag{1.2}$$

with respect to the unknown matrices X and Y with an unknown number of columns k. We determine k from the condition that the unknown reduction of form (1.1) shall consist of the minimum number of terms.

Definition 1. The matrix $Z \in M_{nm}$ is said to be k-reducible if k is the least number for which there are matrices $X \in M_{nk}$ and $Y \in M_{mk}$, satisfying the equation $XY^{\mathrm{T}} = Z$. The ordered pair of matrices (X, Y) is called the k-reduction of Z.

We will denote the set of all k-reductions of Z by M_Z^k.

Lemma 1. The matrix $Z \in M_{nm}$ is k-reducible if, and only if, its rank is equal to k. Any k-reduction consists of matrices of full rank.

Proof. Sufficiency. Let the rank of the matrix Z be k. Then it cannot be q-reducible for $q < k$. On the other hand, Z can be represented in the form of the product of $(n \times k)$- and $(k \times m)$-matrices (skeleton reduction [3]), where the columns of the first can be taken as k linearly independent columns of Z. The matrix Z is k-reducible.

Necessity. Let (X, Y) be any k-reduction of Z. The rank of the matrices X, Y and Z obviously cannot be greater than k. It also cannot be less than k, since otherwise, as we have proved, the matrix Z would be q-reducible for $q < k$. This proves the lemma.

Let (X, Y) be any k-reduction of Z. Then the matrices $X^{\mathrm{T}}X$ and $Y^{\mathrm{T}}Y$ are non-degenerate and (1.2) is equivalent to each of the equations

$$Y = Z^{\mathrm{T}}X\,(X^{\mathrm{T}}X)^{-1}, \quad X = ZY\,(Y^{\mathrm{T}}Y)^{-1}. \tag{1.3}$$

Lemma 2. Let (X, Y) be any k-reduction of the matrix Z. Then the set of all its k-reductions has the form

$$M_Z^k = \{(XA,\ YA^{-1\mathrm{T}}):\ A \in M_{kk},\ \operatorname{rang} A = k\}.$$

Proof. Obviously, any pair of matrices of the given form is a k-reduction of Z. The converse is also true: for any k-reduction (U, V) there is a non-degenerate $(k \times k)$-matrix A such that $U = XA$, $V = YA^{-1\mathrm{T}}$. For, using (1.3), it is easy to check that these equations are true by putting $A = Y^{\mathrm{T}}V(V^{\mathrm{T}}V)^{-1}$. Also, A is non-degenerate, as is seen from the upper and lower bounds of the ranks: $k = \operatorname{rank} U = \operatorname{rank} XA \leq \operatorname{rank} A \leq k$. Thus, the set of this form and the set of all k-reductions of the matrix Z are identical. This proves the lemma.

The following theorem is a direct consequence of Lemmas 1 and 2.

Theorem 1. If the rank of the matrix Z is equal to k, the matrix is k-reducible and

$$M_Z^k = \{(XA,\ YA^{-1\mathrm{T}}):\ A \in M_{kk},\ \operatorname{rang} A = k\},$$

where the matrix X is made up of k linearly independent columns of Z and the matrix Y is defined by the formula $Y = Z^{\mathrm{T}}X(X^{\mathrm{T}}X)^{-1}$.

Thus, with the given definition of an underived surface, for any admissible surface infinitely many different structural descriptions can be indicated. To ensure that the description is unique, additional restrictions must be placed on the set of underived surfaces. This problem will be considered in Section 3.

2. CALCULATING k-REDUCTIONS

According to Lemma 2, the set of all k-reductions is uniquely defined by any one element of the set. The computation of an arbitrary k-reduction of a given matrix is therefore of practical interest. Theorem 1 is not suitable for this purpose, because if the elements of the matrix Z are given with errors, its rank might not be equal to the number of underived surfaces k. A possible way out is to find an approximate solution of the matrix equation (1.2) and determine k from the condition for (1.2) to be satisfied sufficiently accurately (within the errors of Z).

In M_{nm} we will introduce the Euclidean norm

$$\|A\| = \Big(\sum_{i=1}^{n}\sum_{j=1}^{m} a_{ij}^2\Big)^{1/2}, \text{ where } A = [a_{ij}]_{n\times m}.$$

Definition 2. The matrix Z is called k, δ-reducible if k is the smallest number for which there is a k-reducible matrix W such that $\|Z - W\| \leq \delta$. The matrix pair (X, Y) is called a k, δ-reduction of Z if it is a k-reduction of W.

Consider the symmetric non-negative definite matrix ZZ^{T}. All its eigenvalues are concentrated on the segment of the real axis $[0, \|Z\|^2]$, and the corresponding eigenvectors can be chosen so that they form a complete orthonormalized system of vectors in $\mathbb{R}^n$. We now prove the following theorem, which is related to the results of [4] concerning singular reduction of matrices.

Theorem 2. Suppose a matrix $z \in M_{nm}$ and real number $\delta \geq 0$ are given. Let $\lambda_1 \geq \ldots \geq \lambda_n$ be all the eigenvalues of the matrix ZZ^{T}. If k is the smallest number for which the condition

$$\lambda_1 + \ldots + \lambda_k \geq \|Z\|^2 - \delta^2, \tag{2.1}$$

is satisfied, the matrix Z is k, δ-reducible, the best set of k, δ-reductions of Z in the sense of the Euclidean norm having the form

$$\{(XA, Z^{\mathrm{T}}XA^{-1\mathrm{T}}): A \in M_{kk}, \operatorname{rang} A = k\},$$

where the $n \times k$-matrix X is made up of orthonormalized eigenvectors of ZZ^{T}, corresponding to the k largest eigenvalues.

Proof. We will define a functional $J_q : M_{nq} \times M_{mq} \to \mathbb{R}$ by the formula

$$J_q(U, V) = \|Z - UV^{\mathrm{T}}\|^2,$$

assuming that rank U = rank $V = q$, and we will find a matrix pair (U, V) for which J_q is a global minimum. Differentiating J_q with respect to U and V, we obtain a system of normal equations for the given least-squares problem (the necessary conditions for a minimum):

$$U^{\mathrm{T}}(Z - UV^{\mathrm{T}}) = 0, \quad (Z - UV^{\mathrm{T}})V = 0. \tag{2.2}$$

We will show that the matrix $R = V^{\mathrm{T}}VU^{\mathrm{T}}U$ is diagonalizable. Since the matrix $U^{\mathrm{T}}U$ is symmetric and positive definite, there is a non-degenerate matrix $S \in M_{qq}$ such that $S^{-1\mathrm{T}}U^{\mathrm{T}}US^{-1} = E$. Then, since the matrix $SV^{\mathrm{T}}VS^{\mathrm{T}}$ is symmetric and non-degenerate, there is an orthogonal matrix $T \in M_{qq}$ such that $T(SV^{\mathrm{T}}VS^{\mathrm{T}})T^{-1} = \Lambda$, where $\Lambda = \operatorname{diag}(d_1, \ldots, d_q)$ is a diagonal matrix. Let $A = TS$. Then it is easily verified that $ARA^{-1} = \Lambda$, so that by a similarity transformation with non-degenerate transforming matrix A, R is reduced to diagonal form.

In system (2.2) we make the non-degenerate replacement of variables

$$U = XA, \quad V = YA^{-1\mathrm{T}}. \tag{2.3}$$

Then the columns of the new matrices X and Y will be orthogonal:

$$X^{\mathrm{T}}X = E, \quad Y^{\mathrm{T}}Y = \Lambda,$$

and system (2.2) becomes the equivalent system

$$Y = Z^{\tau}X, \quad ZZ^{\tau}X = X\Lambda.$$

The second of these equations means that $d_1, \ldots, d_q$ are eigenvalues, and the columns of the matrix X are the corresponding eigenvectors of ZZ^m.

A sufficient, not merely necessary, condition for a minimum can be obtained by computing the value of the functional J_q^* for U and V that satisfies (2.2). Since $J_q(U, V) = J_q(X, Y)$, we have

$$J_q^* = \mathrm{tr}(Z - XY^{\tau})^{\tau}(Z - XY^{\tau}) = \mathrm{tr}\, ZZ^{\tau} - \mathrm{tr}\, \Lambda = \|Z\|^2 - (d_1 + \ldots + d_q).$$

The global minimum of the functional $J_q(U, V)$ will be reached if, and only if, $d_1, \ldots, d_q$ are the q largest eigenvalues of the matrix ZZ^{τ}. Also, if $q = k$, then by condition (2.1),

$$\|Z - UV^{\tau}\|^2 = J_k^* = \|Z\|^2 - \lambda_1 - \ldots - \lambda_k \leq \delta^2.$$

But if $q < k$, for any $U \in M_{nq}$ and $V \in M_{mq}$,

$$\|Z - UV^{\tau}\|^2 \geq J_q^* = \|Z\|^2 - \lambda_1 - \ldots - \lambda_q > \delta^2.$$

Thus, the matrix Z turns out to be k, δ-reducible, and the k, δ-reductions (U, V) minimize $J_k(U, V)$ if, and only if, they are related by transformation (2.3) with the pair $(X, Z^{\tau}X)$, in which the matrix X is made up of orthonormalized eigenvectors ZZ^{τ}, corresponding to the k largest eigenvalues. This proves the theorem.

According to Theorem 2 a k, δ-reduction of Z can be found if δ is given and the set of eigenvalues and vectors of the matrix ZZ^{τ} is known. However, the computer time needed to find the spectrum increases rapidly with the dimensions of the matrix Z. It is therefore advisable to examine algorithms which do not require the eigenvalue problem to be solved explicitly.

We will investigate the possibility of calculating k, δ-reductions with the help of an iterative process based on relations (1.3).

We will use the following notation. Let $X \in M_{nk}$ be a matrix of rank k. We will denote the linear envelope of the columns of X by $\mathcal{L}(X)$. The projection matrix $P_X = E - X(X^{\tau}X)^{-1}X^{\tau}$, regarded as a linear operator from $\mathbb{R}^n$ into $\mathbb{R}^n$, sets a column-vector in correspondence with its projections on to the orthogonal complement of the subspace $\mathcal{L}(X)$. We then use the following properties of projection matrices.

1. The matrix P_X is symmetric ($P_X^{\tau} = P_X$), idempotent ($P_X P_X = P_X$) and degenerate ($P_X X = 0$, the rank of P_X is equal to $n - k$).

2. The matrix P_X is invariant with respect to the choice of basis in the subspace $\mathcal{L}(X)$: $P_{XA} = P_X$ for any non-degenerate $A \in M_{kk}$.

3. The solution of the following least-squares problem can be expressed in terms of the projection matrix: $\min_X \|AX - B\|^2 = \|P_A B\|^2$.

This last point enables us to define the sine of the angle $\varphi \in [0, \pi/2]$ between subspaces $\mathcal{L}(X)$ and $\mathcal{L}(X_0)$, $X_0 \in M_{nk}$ as the maximum distance from the unit vector of one of the subspaces to the other subspace

$$\sin\varphi = \max_{a \in M_{k,1}} \frac{\|P_X X_0 a\|}{\|X_0 a\|}. \tag{2.4}$$

Theorem 3. Let (X, Y) be the best k, δ-reduction of the matrix $Z \in M_{nm}$ of rank n, in the sense of the Euclidean norm, and let the initial approximation $Y_0 \in M_{mk}$ satisfy the condition $\mathrm{rank}\, Y_0^{\tau}Y = k$, $\lambda_1 \geq \ldots \geq \lambda_n$ are all the eigenvalues of the matrix ZZ^m. Then for the iterative process

$$X_r = ZY_{r-1}A_r, \quad Y_r = Z^{\tau}X_r, \tag{2.5}$$

where the matrices A_r are determined from the conditions $X_r^{\tau}X_r = E$, $r = 1, 2, \ldots$,

$$\|Z - X_r X_r^{\tau}\| \leq \delta + \delta\sqrt{k}\,\mu^{r-1}\,\mathrm{tg}\,\varphi, \tag{2.6}$$

where $\mu = \delta^2\|\Lambda^{-1}\|$, $\Lambda = \mathrm{diag}(\lambda_1, \ldots, \lambda_k)$ and φ is the angle between $\mathcal{L}(X)$ and $\mathcal{L}(X_0)$.

Proof. Since the matrices Z and Y_0 have full rank, for any $r > 0$ the rank of the matrices X_r and Y_r is equal to k. Hence at each iteration there is a non-degenerate upper triangular matrix A_r, defined by the

condition $X_r^T X_r = E$. It can be constructed simply by applying the Gram–Schmidt orthogonalization [3, 4] to the columns of the matrix ZY_{r-1}.

The following identity can be verified by simple reduction:

$$Z - X_r Y_r^T = P_{X_r} Z = P_{X_r} (Z - XY^T) (P_Y - P_Y Y_{r-1} (Y^T Y_{r-1})^{-1} Y^T).$$

We will introduce the notation $Q_r = P_Y Y_r (Y^T Y_r)^{-1} Y^T$, $r = 0, 1, \ldots$. Using (2.5), we will express the matrix Q_r in terms of Y_{r-1}:

$$Q_r = (P_Y Z^T Z P_Y) P_Y Y_{r-1} (Y^T Y_{r-1})^{-1} \Lambda^{-1} Y^T.$$

Since $Y^T Y = \Lambda$ and $\|ZP_Y\| \leq \delta$, for the norm of Q_r we have:

$$\|Q_r\| \leq \|ZP_Y\|^2 \|Q_{r-1}\| \|\Lambda^{-1}\| \leq \mu \|Q_{r-1}\|, \quad r = 1, 2, \ldots$$

When any matrix is multiplied by a projection matrix, its norm can only decrease, and therefore

$$\|Z - X_r Y_r^T\| \leq \delta + \delta \|Q_{r-1}\| \leq \delta + \delta\mu^{r-1} \|Q_0\|.$$

We will now find bounds for the norm of Q_0. Obviously, there are orthogonal $(m \times k)$-matrices $\tilde{Y}$, $\tilde{Y}_0$ and non-degenerate $(k \times k)$-matrices A, A_0 such that $Y = \tilde{Y}A$ and $Y_0 = \tilde{Y}_0 A_0$. Using the identity $\|Q_0\|^2 = \operatorname{tr} Q_0^T Q_0$, we obtain

$$\|Q_0\|^2 \leq \operatorname{tr} (\tilde{Y}_0^T \tilde{Y} \tilde{Y}^T \tilde{Y}_0)^{-1} - \operatorname{tr} \tilde{Y}^T \tilde{Y} \leq k/\lambda - k,$$

where λ is the smallest eigenvalue of the matrix $G = \tilde{Y}_0^T \tilde{Y} \tilde{Y}^T \tilde{Y}_0$. Since the matrix G is symmetric and positive definite,

$$\lambda = \min_a \frac{a^T G a}{a^T a}.$$

Making the substitution $\tilde{Y}\tilde{Y}^T = E - P_Y$ in G, using (2.4) we find

$$\lambda = 1 - \max_a \frac{\|P_Y Y_0 a\|^2}{\|Y_0 a\|^2} = \cos^2 \varphi.$$

Notice that $\cos \varphi \neq 0$, since the matrix $Y_0^T Y$ is non-degenerate. Thus,

$$\|Q_0\| \leq \sqrt{\frac{k}{\cos^2 \varphi} - k} = \sqrt{k} \operatorname{tg} \varphi,$$

whence the required inequality follows at once. This proves the theorem.

The estimate (2.6) shows that if the error of the initial data is sufficiently small, the procedure (2.5) achieves acceptable accuracy even at the first iterations. In particular, if the initial matrix is k-reducible ($\delta = 0$), the equation $Z = X_1 Y_1^T$ is satisfied exactly for any Y_0 satisfying the condition $\operatorname{rank} Y_0^T Y = k$.

Notice that if the matrices A_r are upper triangular, any number of iterations can be performed on the first q columns of the matrices X and Y without having to know the other $k - q$ columns. This gives a more flexible algorithm, in which iterations with respect to r are alternated with the addition of new columns to the matrices X_r, Y_r. To be more precise, after adding a new (qth say) column to the matrix Y_0, we compute the qth columns of the matrices X_1, Y_1, X_2, Y_2, and so on. The addition of columns must be stopped as soon as the error (2.6) becomes less than a given value d after a sufficient number of iterations N. Thus, this modification of the procedure (2.5) enables the number k to be determined from the condition that the reduction has reached the prescribed accuracy. We now write this algorithm in a form that can be implemented on a computer. We will use the notation

$$Z \equiv [z_1 \ldots z_m] \in M_{nm}, \quad X_q^r \equiv [x_1^r \ldots x_q^r] \in M_{nq}, \quad P_q^r \equiv P_{X_q^r}, \quad P_0^r = E,$$

$$r = 1, 2, \ldots, N;$$

$$Y_q^r \equiv [y_1^r \ldots y_q^r] \in M_{mq}, \quad h_0, \ldots, h_q \in M_{m,1}, \quad r = 0, 1 \ldots, N, \quad q \geq 1.$$

Algorithm

Input. $Z \in M_{nm}$, accuracy $d \geq 0$, number of iterations $N > 0$.
Step 1. $H_0 := \|Z\|^2$.
Step 2. $h_{j0} := \|z_j\|^2$ for all $j = 1, 2, \ldots, m$.
Step 3. For $q = 1, 2, \ldots$, repeat steps 4–10.
Step 4. $y_q^0 := h_q$.
Step 5. For $r = 1, 2, \ldots, N$, repeat steps 6–7.
Step 6. $x_q^r := P_{q-1}^r Z y_q^{r-1} / \|P_{q-1}^r Z y_q^{r-1}\|$.
Step 7. $y_q^r := Z^T x_q^r$.
Step 8. $h_{jq} := h_{jq-1} - (y_{jq}^N)^2$ for all $j = 1, 2, \ldots, m$.
Step 9. $H_q := H_{q-1} - \|y_q^N\|^2$.
Step 10. Continue for as long as $H_q > d^2$.
Result: $(X_q^N, Y_q^N): \|Z - X_q^N (Y_q^N)^T\| \leq d$, X_q^N has been orthonormalized.

It is not guaranteed that the matrix pair (X_q^N, Y_q^N) found by this algorithm will be a q, d-reduction of Z, since in the general case the number of columns q cannot satisfy the minimality condition. However, it is clear from the following assertion that, by the suitable choice of the parameters of the algorithm N and d, one k, d-reduction of the matrix Z can be determined.

Assertion. Suppose that all the conditions of Theorem 3 are satisfied and $\mu < 1$. Then for any $\varepsilon \in (0, \lambda_k)$, there is a natural number N_0 such that, for $d^2 = \|Z - XY^T\|^2 + \varepsilon$ and $N \geq N_0$, the matrix pair computed by the algorithm will be a k, d-reduction of Z.

Proof. It is easily verified (cf. Steps 1 and 9) that $H_q \equiv \|Z - X_q^N (Y_q^N)^T\|^2$, $q = 1, 2, \ldots$. Hence, the termination condition of the algorithm (Step 10) cannot be satisfied for $q < k$, since otherwise, according to Theorem 2, ε would have to be greater than λ_k. On the other hand, by using (2.6) to express the iteration number r, for $q = k$ and

$$N \geq 1 + (\ln \mu)^{-1} \ln \left[\frac{1}{\operatorname{tg} \varphi \sqrt{k}} \left(\sqrt{1 + \varepsilon / \partial^2} - 1 \right) \right]$$

the termination condition will be satisfied and the matrix pair (X_q^N, Y_q^N) obtained by then will be a k, d-reduction of Z. This proves the assertion.

Thus, for a suitable choice of the number of iterations N and threshold d, it is possible to determine one of the k, d-reductions of Z. In practice, it turns out that if we put $N = 2$–4 and $d = (1.2$–$1.6)\,\delta$, then with very rare exceptions, the matrices X_q^N, Y_q^N will not contain superfluous columns.

We note that if $k << \min(n, m)$, the algorithm can be used to compress the initial data efficiently by replacing the matrix Z by a pair of matrices of much smaller size. This enables large teaching samples to be stored even when the memory is limited.

3. OPTIMAL k-REDUCTIONS

In order to ensure that the description of an admissible surface that is sought is unique, we need to solve the regularization problem, imposing additional constraints on the set of underived surfaces. The a priori information used for this purpose must satisfy two conditions. Its use must be justified in the framework of the problem to be solved, and it must be sufficient for one to be able to identify a unique solution from the infinite set of solutions.

Consider the following method of taking account of a priori information. Only those functions of the form $f(x)\,g(y)$ that will be put in the class of underived surfaces are those for which $f(x)$ belongs to the prescribed family of functions $\mathcal{F}$. As before $g(y)$ can be any function.

For a fixed set of n numbers $\xi_i \in \Omega_x$, $i = 1, 2, \ldots, n$, the family $\mathcal{F}$ induces the set of column vectors

$$\mathcal{F}_n = \{|f(\xi_1) \ldots f(\xi_n)|^T : f \in \mathcal{F}\}$$

and the set of $n \times k$ matrices with columns from $\mathcal{F}_n$

$$\mathcal{F}_{nk} = \{|u_1 \ldots u_k| : u_s \in \mathcal{F}_n,\ s = 1, 2, \ldots, k\}.$$

Let (X, Y) be a known k-reduction of the matrix Z, and for simplicity let the columns of X be orthonormalized, $X^TX = E$. The problem is to determine the conditions which must be satisfied by the

family $\mathcal{F}$ for there to be a unique matrix $U \in \mathcal{F}_{nk}$ (unique apart from permutation of the columns), such that $\mathcal{L}(X) = \mathcal{L}(U)$, and also to find a way of computing this matrix.

Definition 3. The family of functions $\mathcal{F}$ is said to be k-non-linear with respect to the set of points $(\xi_1, \ldots, \xi_n)$, if for any pairwise different column-vectors $u_0, \ldots, u_k$ of the set $\mathcal{F}_n$ and any real $a_1, \ldots, a_k$, $a_1u_1 + \ldots + a_ku_k \neq u_0$.

There are families of functions which possess this property. For instance, the parametric family $\mathcal{F}^{\alpha} = \{e^{-(x-\alpha)^2} : \alpha \in \mathbb{R}\}$ is k-non-linear with respect to any set of n different points for all $k = 1, 2, \ldots, n-1$. To prove this, we form a $[n \times (k+1)]$-matrix of arbitrary pairwise-different column-vectors $u_0, \ldots, u_k$ belonging to the set $\mathcal{F}_n^{\alpha}$. By virtue of the identity $e^{-(x-\alpha)^2} = e^{-x^2}e^{2x\alpha}e^{-\alpha^2}$, its first $k+1$ rows form a square matrix, which can be obtained by multiplying the rows and columns of the generalized Vandermonde matrix [3] by positive numbers. The determinant of that matrix is non-zero. Hence, the column-vectors $u_0, \ldots, u_k$ are linearly independent, and since they are arbitrary, the given family is k-non-linear.

There are also families which do not possess the given property. In particular, any linear family of functions, such as the set of polynomials of given degree, cannot be k-non-linear. It will become clear that such families of functions cannot be used for regularization.

Definition 4. The family of functions $\mathcal{F}$ is called k-correct with respect to the set of points $(\xi_1 \ldots \xi_n)$ for a given matrix $X \in M_{nk}$ of rank k if there is a non-degenerate $(k \times k)$-matrix A such that $XA \in \mathcal{F}_{nk}$.

Theorem 4. If $\mathcal{F}$ is a family of functions which is k-non-linear and k-correct with respect to the set of points $(\xi_1 \ldots \xi_n)$ for a given matrix X, there is a unique matrix $U_* \in \mathcal{F}_{nk}$ (apart from permutation of the columns) such that $\mathcal{L}(U_*) = \mathcal{L}(X)$.

Proof. By virtue of the k-correctness of the family $\mathcal{F}$ in the subspace $\mathcal{L}(X)$ there are k linearly independent column vectors $u_1^*, \ldots, u_k^*$ belonging to $\mathcal{F}_n$. By virtue of k-non-linearity, there cannot be any other elements $\mathcal{F}_n$ in $\mathcal{L}(X)$. Hence, the matrices $U \in \mathcal{F}_{nk}$ satisfy the condition $\mathcal{L}(X) = \mathcal{L}(U)$ if, and only if, they are made up of column vectors $u_1^*, \ldots, u_k^*$ taken in any order. This proves the theorem.

It is clear from the proof that k-non-linearity ensures uniqueness, and k-correctness ensures the existence of a regularized solution.

In practice it is impossible to guarantee that the subspaces $\mathcal{L}(X) = \mathcal{L}(U)$ coincide exactly for many reasons: because of the errors of the initial data or the errors in computing the matrix X and, most importantly, the inaccuracy of the description of underived surfaces by elements of the family. We will therefore relax the condition for k-correctness: we will seek a matrix $U_* \in \mathcal{F}_{nk}$ for which the functional

$$\bar{J}(U) = \|P_U X\|^2,$$

which vanishes if, and only if $\mathcal{L}(X) = \mathcal{L}(U)$, reaches a minimum. Thus, minimization of the matrix must lead to the required solution in the case of k-correct families.

We will orthonormalize the columns of the matrix $U \equiv [u_1 \ldots u_k]$, applying to them the Gram–Schmidt procedure, and denote the resulting matrix by $\tilde{U} \equiv [\tilde{u}_1 \ldots \tilde{u}_k]$. We will determine the sequence of projection matrices

$$P_1 = E_n, \quad P_s = P_{\tilde{u}_1} \ldots P_{\tilde{u}_{s-1}} \equiv E - \tilde{u}_1\tilde{u}_1^{\mathrm{T}} - \ldots - \tilde{u}_{s-1}\tilde{u}_{s-1}^{\mathrm{T}}, \quad s = 2, 3, \ldots, k.$$

Then

$$\tilde{u}_s = P_s u_s / \|P_s u_s\|, \qquad s = 1, 2, \ldots, k.$$

Owing to the elementary properties of a Euclidean matrix norm

$$\bar{J}(U) = \|P_X \tilde{U}\|^2 = \sum_{s=1}^{k} \frac{\|P_X P_s u_s\|^2}{\|P_s u_s\|^2}.$$

We note that $P_X P_s = P_X$ in the case of k-correctness, and thus the functional $\bar{J}(U)$ can be replaced by its upper bound

$$J(U) = \sum_{s=1}^{k} \frac{\|P_X u_s\|^2}{\|P_s u_s\|^2}, \tag{3.1}$$

without violating the condition $J(U) = 0 \Leftrightarrow \mathcal{L}(X) = \mathcal{L}(U)$. We will introduce notation for the terms in (3.1)

$$J_s(u) \equiv J_s(u_1, \ldots, u_{s-1}, u) \equiv \|P_X u\|^2 / \|P_s u\|^2, \quad s = 1, 2, \ldots, k, \tag{3.2}$$

and consider the sequence of minimizations

$$u_s^* = \arg\min_{u \in \mathcal{F}_n} J_s(u_1^*, \ldots, u_{s-1}^*, u), \quad s = 1, 2, \ldots, k. \tag{3.3}$$

If the family $\mathcal{F}$ satisfies the conditions of Theorem 4, the successive minimization (3.3) leads to the required minimum of the functional $J(U)$. For, by virtue of k-correctness, there is a set of different vectors $u_1^*, \ldots, u_k^*$ which make the functionals $J_1, \ldots, J_k$, respectively, zero. Due to k-non-linearity, this set is unique, and the vectors in it are linearly independent. The matrix U_* formed from these vectors is the unique matrix (apart from permutation of the columns) which makes the functional $J(U)$ a minimum, equal to zero.

Thus, the minimization of $J(U)$ with respect to the set $\mathcal{F}_{n,k}$ can be reduced to the much simpler problem of successive minimization of the functionals $J_1, \ldots, J_k$ over the set $\mathcal{F}_n$.

In the general case, when the minimum of $J(U)$ is not equal to zero (there is no k-correctness), one can speak only of approximate minimization with the help of (3.3). It is clear, however, that the better the family $\mathcal{F}$ describes the functions $f(x)$, the closer the minimum of the functional $J(U)$ is to zero, and the closer the matrix U_* computed with the help of (3.3) is to the matrix which minimizes $J(U)$. Whether or not the condition of k-correctness is satisfied, the concept of an optimal k-reduction can be introduced.

Definition 5. The optimal k-reduction is the matrix pair $(X_0, Y_0) \in M_Z^k$ for which the functional

$$\Phi(\tilde{X}, \tilde{Y}) = \|\tilde{X} - U_*\|, \quad (\tilde{X}, \tilde{Y}) \in M_Z^k,$$

is a minimum, where U_* is the matrix computed by the algorithm (3.1)–(3.3).

It is easy to obtain formulae to calculate the optimal k-reduction by minimizing Φ with respect to the set M_Z^k and using Lemma 2:

$$X_0 = XX^T U_*, \quad Y_0 = Y(U_*^T X)^{-1}.$$

We will consider two special cases.

Case 1. For the teaching of pattern recognition [1, 2], the family $\mathcal{F}$ can be taken as a finite set of l functions $F_1(x), \ldots, F_l(x)$, forming the underived elements of admissible surfaces of objects of the teaching sample (l is the sample length). In that case, minimization of each of the functionals J_s in (3.2) reduces to a linear examination of l elements of the set $\mathcal{F}$.

It is taken for granted in this approach that the following hypothesis is accepted: "the function $f(x)$ of an underived element of an admissible surface of the object to be classified is equal, or at least, very close to one of the functions $F_1(x), \ldots, F_l(x)$". Clearly, if only one teaching sample is used to solve the regularization problem, the sample might have to be longer than could be justified merely on teaching grounds.

Case 2. Let $\mathcal{F} = \{f(x, \alpha) : \alpha \in \mathbb{R}^p\}$ be a parametric family of functions satisfying the conditions of Theorem 4. Minimization of the functionals $J_1, \ldots, J_k$ in (3.3) will obviously reduce to the minimization of k functions of p variables over the set of admissible values of the parameters. The well-known optimization methods [5] can be used to solve the problem, the initial approximations conveniently being taken as the approximations of the functions $F(x)$ of underived elements chosen from the teaching sample. One could use algorithm (3.1)–(3.3) to pick out the k most suitable teaching objects for this purpose, as before.

Hence, by restricting the set of underived surfaces by a priori assignment of a family of functions which corresponds to the specific accuracy and non-linearity conditions, and then computing the optimal k-reduction, one can identify the unique structural description of the original admissible surface and thereby solve the problem.

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