Construction of separating function for objects classification and its use for classification of spherical segments from material with shape memory

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Abstract. An engineering method for constructing a separating surface for discriminating classes of multiparameter objects is described. The method is based on the proposed approximation of the membership function, which makes it possible to classify with a complex form of the separating surface. An algorithm is given for calculating the estimates of the coefficients of the nonlinear model with respect to the coefficients of the separating surface model using an iterative procedure based on the method of least squares. The results of experiments and calculations on the classification of spherical segments from materials with shape memory, proving the effectiveness of the proposed method are presented.

1. Approach to classification
There is a wide class of problems in which it is necessary to determine regions belonging to different classes by a certain criterion for multiparameter objects in the space of their parameters

\[ X = \{x_1, x_2, \ldots, x_m\}^T. \]

Selection of such areas allows you to determine the properties of the objects that provide a given class. Such a problem arises, for example, when determining the optimal geometric parameters of segments from materials with shape memory for different classes by the presence of a rebound [1]. Usually in practice, the number of parameters is large enough and the classes are intermixed, so mathematical-statistical methods are used to distinguish the classes [2].

However, the formal use of such methods often does not allow us to separate classes with sufficient accuracy for practice, since the interfaces between classes are usually quite complex, and their form is unknown. For example, the use of Fisher's discriminant for constructing a class separating classes leads to large class definition errors due to insufficient information about the distribution of components for each class. In these conditions, it is proposed to use the method of least squares to construct the separating surface [3, 4].

2. Classification problems and methods to solve them
In accordance with this method of estimating the coefficients \( B \), separating classes surface \( g(X, B) = 0 \) are constructed so that they provide a minimum of the sum of the squares of the deviations in the form [5]

\[
\sum_{i=1}^{n} \left[ g(X, B) - y_i \right]^2 = \min_B \left\{ \sum_{i=1}^{n} \left[ g(X, B) - y_i \right]^2 \right\}, \quad (1)
\]
where \( g(X, B) \) is the separating function, \( X = \{x_1, x_2, \ldots, x_n\}^T \) is the vector of parameters, \( B = \{b_1, b_2, \ldots, b_l\}^T \) is the coefficient estimation vector, \( y \) is the attribute of belonging to the given class (for example, \( y = 1 \) if the object belongs to the first class by test results, and \( y = -1 \), second class), \( n \) is the sample size.

However, with this approach, contributions to the sum of deviations (1) will be produced by objects with large values of the separating function \( g(X, B) \), which leads to significant errors in class recognition, especially in the complex form of the classifying function, which is typical for technical applications.

### 3. The method of constructing a separating surface for two classes

For a objects, there is a probability of belonging to the class defined \( q_1 \) and the probability of belonging to an alternative class (\( q_2 \) (\( q_1 + q_2 = 1 \)). Experimentally, belonging to this class (\( y = 1 \)) or not belonging to this class (\( y = -1 \)) is determined by the results of testing objects that give an estimate of the value of the membership function \( q(X) = q_1 - q_2 \) as a function of the magnitude of the component vector. As a result of testing of \( n \) articles, the evaluation of the membership vector is determined \( Y = \{y_1, y_2, \ldots, y_n\}^T \).

Approximation of the dependence of the magnitude \( q \) on the values of the parameters is proposed to be presented in the form [6]:

\[
q(X, B) = \text{sign}[f(X, B)] - \exp[\frac{1}{2} f(X, B)^2],
\]

where \( f(X, B) \) is some function whose form and coefficients are determined from the experimental data.

Function (2) is equal to zero on the interface between two classes and tends to 1 (or -1) when moving away from the separating surface. The separating surface is defined by the equation

\[
q(X, B) = 0.
\]

In this case, the calculation of the coefficient estimates in expression (3) by the least squares method is performed using the following iterative procedure [7,8]:

\[
B^{s+1} = B^s + \left[ \sum_{i=1}^{n} P(X_i, B^s) P^T(X_i, B^s) \right]^{-1} \sum_{i=1}^{n} P(X_i, B^s) \left[ y_i - q(X_i, B) \right],
\]

where \( s \) is the iteration number.

\[
P(X, B) = \frac{\partial q(X, B)}{\partial B} = \text{sign}[f(X, B)] \exp[\frac{1}{2} f(X, B)^2] \frac{\partial f(X, B)}{\partial B},
\]

and \( \frac{\partial f(X, B)}{\partial B} = \left\{1, x_1, x_2, \ldots, x_1, x_2, \ldots, x_1, x_2, \ldots, x_3 \right\}^T \) for a complete quadratic function.

The covariance matrix for estimating the coefficients (4) is calculated by formula

\[
V_B = \sigma^2 \cdot \left[ \sum_{i=1}^{n} P(X_i, B) P^T(X_i, B) \right]^{-1},
\]

where \( \sigma^2 \) is the variance of the class recognition error.

As an estimate of the variance of class recognition, the variance of the model’s adequacy error is calculated, by formula:

\[
\sigma^2 = \frac{1}{n - l} \sum_{i=1}^{n} \left[ q(X_i, B) - y_i \right]^2,
\]

where \( l \) is the number of coefficients in the model (2).
The diagonal elements of matrix $V_\alpha$ (6) represent the variances of the estimates of the corresponding coefficients, which makes it possible to calculate their t-statistics and, therefore, to check the significance of the coefficient estimates.

The lower boundary of the one-way confidence interval for the separating function that ensures the probability of recognizing the first class is not less than $P\%$ is defined as:

$$q(X, B) = q(X, B) - t_{P, f} \sigma_x,$$

where $t_p$ is the Student's distribution quantile for the probability $P$ and the number of degrees of freedom $f$, $B$ is the coefficient estimations vector.

4. Construction of the model of the dependence of impact force of spherical segments from material with shape memory from geometric parameters

The described procedure for constructing a separating function was used to classify spherical segments from material with shape memory according to the classes of magnitude of the rebound strength when using different geometric dimensions. Experimentally obtained data on the dependence of the impact force of spherical segments on their geometric dimensions were processed by regression analysis [3]. As a model describing the dependence of the impact force of a segment on the obstacle on the ratio of geometric parameters $D/R$ and $h/R$, we used the quadratic function in form

$$P_\alpha = b_0 + b_1 z_1 + b_2 z_2 + b_{12} z_1 z_2 + b_{11} z_1^2 + b_{22} z_2^2,$$

where $z_1$ and $z_2$ are independent variables, $z_1=D/R$ and $z_2=h/R$, $P_\alpha$ is the specific impact force with a clap (kg).

The coefficients of the model $b_0$, $b_1$, $b_2$, $b_{12}$, $b_{11}$ and $b_{22}$ were determined by the method of least squares [9,10]. The significance of the coefficients $b_i$ was checked according to the $t$-criterion [9], when the $t$-statistics in form $t_i = |b_i| / s_{bi}$ is compared with the student's Student's distribution quantile for a given number of degrees of freedom $f=n-k$, where $n$ is the number of experiments, $k$ is the number of coefficients in the model, significance level (the significance level was assumed to be 0.05). Estimates of the coefficients of model (9) and the values of $t$-statistics are given in Table 1.

| $b_i$ | $b_0$ | $b_1$ | $b_2$ | $b_{12}$ | $b_{11}$ | $b_{22}$ |
|------|-------|-------|-------|---------|---------|---------|
|      | 30.8  | -270.8| 7522.8| -32407.5| 613.2   | 432437.1|
| $t_i$| 1.556 | -3.455| 4.182 | -5.098  | 5.247   | 4.312   |

A coefficient is assumed to be insignificant at the level of significance $\alpha$ if inequality is valid,

$$t \leq t_{f,1-\alpha},$$

where $t_{f,1-\alpha}$ is the Student's distribution quantile for the probability $1-\alpha$ with the number of degrees of freedom $f=n-k$, $n$ is the number of observations, $k$ is the number of coefficients in the model equation.

In this experiment, $n = 72$ and $k = 6$ for model (9), then $f = 66$ and with the Student's quantile distribution $t_{f,1-\alpha} = 1.67$. From Table 1 it follows that the coefficient $b_0$ is insignificant, so the corresponding term is excluded from equation (9); the values of the coefficient estimates are recalculated for an equation with five coefficients in form

$$P_\alpha = b_1 z_1 + b_2 z_2 + b_{12} z_1 z_2 + b_{11} z_1^2 + b_{22} z_2^2.$$

The estimates of the coefficients $b_i$ calculated for equation (11) and the corresponding values of the $t$-statistics (10) are given in Table 2.
Table 2. The estimates of the coefficients $b_i$.

| $b_1$ | $b_2$ | $b_{12}$ | $b_{21}$ | $b_{22}$ |
|-------|-------|----------|----------|----------|
| -174.0 | 6922.9 | -31595.3 | 538.8    | 432726   |

In this case, $f = 67$ and $t_{f,1-a} = 1.67$. From Table 2 it is clear that all the coefficients are significant.

Thus, the calculation of the strength of clap is carried out in accordance with the expression (3), the coefficients $b_i$ of which are presented in Table 2.

To check the adequacy of the constructed model (10), the residual dispersion $s_r^2$ was calculated by formula:

$$ s_r^2 = \frac{1}{f} \sum_{j=1}^{n} (P_{yvj} - P_{ypp})^2 $$  \hspace{1cm} (12)

where $P_{yvj}$ is the evaluation of the strength of the impact, obtained from the expression (3) for the $j$-th observation, $P_{ypp}$ is the corresponding observed value of the strength of impact, $f$ is the number of degrees of freedom.

For model (11), the residual dispersion (12) is equal to $s_r^2 = 2.847 \text{ kg}^2$. For the model constructed in [4] for the geometric parameters $D/R$ and $h/R$, the residual dispersion has the value $s_r^2 = 9.07 \text{ kg}^2$, i.e. model (11), which uses the $D/R$ and $h/R$ ratios, agrees much better with the experimental data.

After substituting the calculated coefficients into equation (11), expression is obtained that describes the dependence of the impact force of a spherical segment on the impeding body on the ratios of the geometric parameters $D/R$ and $h/R$, in form

$$ P_{y} = -174 \cdot \frac{D}{R} + 6922.9 \cdot \frac{h}{R} - 31595.3 \cdot \frac{D}{R^2} + 538.8 \cdot \left( \frac{D}{R} \right)^2 + 432726 \cdot \left( \frac{h}{R} \right)^2. $$  \hspace{1cm} (13)

Our studies show that not all combinations of the parameters $D/R$ and $h/R$ realize clapping and hitting conditions and on obstructive body. In this connection, it is of interest to construct the separating function in the coordinate system $D/R$ and $h/R$, which allows us to divide the regions where the impact on the obstructive body takes place and in which it is absent.

5. Construction of separating function

Analysis of the experimental data on the strength of the impact, depending on the ratio of the $D/R$ and $h/R$ segments, showed that the segments clapping with clap and impact against the interfering body (force-measuring device) are concentrated within a certain closed region (Figure 1) restoring the form without impact, are beyond the boundaries of this area.
Figure 1. The scattering field for the geometric parameters of segments and the form of the separating function (circles—with impact, crosses - without).

To determine the range of the variables (\(z_1\) and \(z_2\)) that provide the real clap of the segment with impact, it is necessary to construct the separating function \(g(Z,A)\). As the separating function \(g(Z,A)\), a second-order function is chosen in form

\[
g(Z,A) = a_0 + a_1 z_1 + a_2 z_2 + a_3 z_1 z_2 + a_4 z_1^2 + a_5 z_2^2,
\]

where \(Z = \left(\frac{D}{R}, \frac{h}{R}\right)^T\) is the vector of geometric parameters \(z_1, z_2\); \(A = \{a_0, a_1, a_2, a_3, a_4, a_5\}^T\) is the coefficient vector.

The calculation of the separating function was carried out by the method of least squares [3]. For segments with an impact on the obstacle, the separating function takes positive values, and for segments without impact - negative. To calculate the estimates of the coefficients \(A\), the values of +1 and -1 for the segments without impact were taken as the observed value of the function \(g(Z,A)\) for the impacted segments. However, the further the segments in the \(D/R\) and \(h/R\) coordinate systems are from the region boundary, the larger the calculated value of the function \(g(Z,A)\), which leads to large errors in the construction of the function \(g(Z,A)\). To limit the influence of segments that are far from the interface on the value of the separating function \(g(Z,A)\) when calculating the coefficients \(A\), equation (14) was transformed by using instead the logarithm function of the module of this function \(h(Z,A)\) with the corresponding sign as follows:

\[
h(Z,A) = \text{sign}[g(Z,A)] \ln\left(|g(Z,A)| + 1\right),
\]

or in the elemental form

\[
h(Z,A) = \text{sign}[g(Z,A)] \ln\left\{a_0 + a_1 \frac{D}{R} + a_2 \frac{h}{R} + a_3 \frac{D h}{R^2} + a_4 \left(\frac{D}{R}\right)^2 + a_5 \left(\frac{h}{R}\right)^2 + 1\right\},
\]
where \( \text{sign}(x) = 1 \) for \( x \geq 0 \) and \( \text{sign}(x) = -1 \) for \( x < 0 \), \( |g(Z, A)| \) is the modulus of the function \( g(Z, A) \).

The term +1 provides positive values of the function for positive values of the function.

Function \( h(Z, A) \) is non-linear with respect to the coefficients, so the coefficients are calculated iteratively. Calculation of estimates of the coefficients \( A \) of equation (6) was carried out with the help of the following iterative procedure [5]:

\[
A^{t+1} = A^{t} + \left[ \sum_{j=1}^{n} F(Z, A)F(Z, A)^{T} \right]^{-1} \sum_{j=1}^{n} F(Z, A)^{T} [u_{j} - h(Z, A)] ,
\]

where \( u_{j} \) is the observed value of the coefficient estimates.

The covariance matrix of the coefficient estimates is calculated by the formula

\[
V_{A} = s^{2} \left[ \sum_{j=1}^{n} F(Z, A)F(Z, A)^{T} \right]^{-1},
\]

where \( s_{t}^{2} \) is the variance of the observation error.

As an estimate of variance in the observation of classes, the residual variance calculated using formula:

\[
s_{t}^{2} = \frac{1}{n-k} \sum_{j=1}^{n} [h(Z, A) - u_{j}]^{2},
\]

where \( k \) is the number of coefficients in the model (14) (in this case, \( k = 6 \)).

The diagonal elements of the matrix \( V_{A} \) (17) represent the variances of the estimates of the corresponding coefficients, which makes it possible to calculate their \( t \)-statistics and, thus, to verify the significance of the coefficient estimates.

The experimental data for calculating the separating function included 72 segments with clap and 65 segments without clap (a total of 137 segments). To calculate the estimates of the coefficients of the separating function from formula (7), a computer program was developed. The results of calculating the estimates of the coefficients of the separating function and \( t \)-statistics are given in Table 3.

| \( a_{i} \) | \( a_{0} \) | \( a_{1} \) | \( a_{2} \) | \( a_{12} \) | \( a_{11} \) | \( a_{22} \) |
|---|---|---|---|---|---|---|
| \( t_{i} \) | -36.51 | 163.17 | -2268.13 | 14494.10 | -301.87 | -215519.28 |
| \( t_{i} \) | 10.46 | 13.06 | -9.94 | 19.50 | -19.40 | -18.54 |

The number of degrees of freedom is \( f = 131 \). In this case the quantile of the Student's distribution is equal to \( t_{f,1-\alpha} = 1.978 \) at the significance level \( \alpha = 0.05 \). Thus, all the coefficients in Table 3 are significant.

When equation (15) is used with the coefficients given in Table 3, it turned out that seven segments hit the segment class without impact, with impact, i.e. are not recognized correctly.

For practical applications of segments, it is important that the segments are recognized correctly without impact. To reduce the error of segment recognition without impact, the observed values of the
function $h(Z, A)$ were assumed with some weight. The higher this weight, the more precisely the segments of the corresponding class are identified.

It was empirically established that with the observed value of the function $h(Z, A) = -2.5$ for segments without impact, all such segments are identified correctly (it can be shown that this corresponds to the probability of incorrect segment recognition without impact, equal to 0.01). After that, the coefficients of the separating function were recalculated. Table 4 shows the results of calculating the coefficients and $t$-statistics for this case.

**Table 4.** The results of calculating the coefficients.

| $a_1$ | $a_2$ | $a_3$ | $a_4$ | $a_5$ | $a_6$ |
|-------|-------|-------|-------|-------|-------|
| -99.00 | 358.35 | -3502.02 | 27422.56 | -601.85 | -425168.92 |
| -28.33 | 27.89 | -13.47 | 33.82 | -35.75 | -32.69 |

Figure 2 shows the form of the separating function. The inner area in Figure 4 is the area of acceptable values of the geometric parameters of the segments at which snapping with impact is realized.

6. **Calculation of optimal values of geometric parameters**

The specific impact strength $P_{sp}$ for the given geometric parameters $D/R$ and $h/R$ was calculated from the model (3) for segments that were within the allowed range. Optimum values of geometric parameters were determined by the method of statistical tests. The program developed for this calculation performs the following actions:

1. generation of geometrical parameters of the segment $D/R$ and $h/R$ in the specified range;
2. checking the belonging of a segment to a class with a impact determined by inequality $g(Z, A) > 0$; if this inequality is not satisfied, then return to item 1;
3. calculation of the impact force $P_{sp}$ for the specified geometric parameters $D/R$ and $h/R$ according to the model (13);
4. remembering the greatest value of the impact force $P_{sp}$ and the corresponding values of the geometric parameters $D/R$ and $h/R$;
5. items 1-4 are repeated predetermined number of times.

Optimization can be performed under given constraints on geometric parameters. To do this, in step 1, for example, you can set the value of $D/R$ and the optimization will be performed for this value.

When finding the optimal parameters, $10^5$ statistical tests were performed, the accuracy of determination of $P_{sp}$ and parameters was $1.1 \times 10^{-4}$. The dependence of the impact force $P_{sp}$ on the parameters $D/R$ and $h/R$ obtained as a result of this calculation is shown in Figure 2.
Figure 2. Type of separating function and modeled impact force values (kg) for various parameters $D/R$ and $h/R$.

In Figure 2 numbers show the calculated values of the impact force for different values of $D/R$ and $h/R$. The black point shows the position of the maximum impact force without any restrictions on geometric parameters. The greatest values of the impact force are in the lower right side of the interface, i.e. at the edge of the allowable area in which clap with impact is performed. The maximum value of the impact force is at the point $h/R=0.024$ and $D/R=0.79$; the force being equal to $P_{p,max}=14.6$ kgf.

Thus, using the form of the separating function, it is not difficult to choose the relations of geometrical parameters ($D/R$ and $h/R$), at which the impact on the obstacle with the strongest force, or close to it, is performed.

In this model, the diameter of the segment is taken equal to 17 mm. Therefore, if in addition to the diameter $D$, the thickness $h$ of the plate is given, then a constant value of the ratio $D/h$ is provided in the program calculation. For example, given $D=16.5$ mm and $h=0.4$ mm, we obtain the values $D/R=0.80$ mm and $h/R=0.019$ mm; at these values, the impact force is 12.66 kgf. The resulted calculation results allow to optimize geometrical parameters of spherical segments.

7. Conclusion

The method for constructing separating function for classification of objects with class mixing based on the method of least squares is developed. This method allows one to build a separating function based on experimental data and use it to determine whether objects belong to a particular class.

The model of the dependence of the impact force on the geometrical parameters of the spherical segments ($D/R$ and $h/R$) allows us to estimate the impact force of the segment on the obstructing body. The model will allow one to determine the geometrical parameters of segments to obtain the greatest impact force.

The constructed separating function in the space of geometrical parameters $D/R$ and $h/R$, allows to determine the regions of geometric parameters of spherical segments from a material with shape memory with impact on obstructing body and without impact. This function enables geometric parameters to identify segments in which the impact is not realized.
The obtained calculations by the model are in good agreement with the experimental results, which makes it possible to determine the optimal sizes of the spherical segments, which ensure the impact of the maximum force.

References
[1] Popov S. A., Khusainov M.A. Bondarev A.B. Andreev V.A., 2005 Vestn. Novgorod. Gos. Univ. 2 (34) 12–16
[2] Popov S. A., Andreev V.A., Khusainov M.A. Bondarev A.B. 2006 Vestn. Novgorod. Gos. Univ. 2 (39) 28–30
[3] Khartman K. 1977 Experiment Design in Investigation of Technological Processes Moscow, "Mir" 552
[4] Bard Y. 1974 Nonlinear Parameter Estimation Academic Press, New York 349
[5] Popov S. A., Andreev V.A. 2006 Vestn. Novgorod. Gos. Univ. 2 (39) 27–32
[6] Popov S. A., Zhizhin V.V. 2007 Vestn. Novgorod. Gos. Univ. 2 (44) 11–13
[7] Popov S. A., Zhizhin V.V. 2009 Vestn. Novgorod. Gos. Univ. 2 (50) 69
[8] Popov S. A. 2010 Zavodskaya Laboratoriya. (4) 40-42
[9] Khusainiv M.A., Popov S. A. Bondarev A.B. 2012 Vestn. Novgorod. Gos. Univ. 2 (67) 38-40
[10] Khusainiv M.A.Popov S. A., Malukhina O.A. 2015 Journal of Applied Physics 2015. (8) 46-52