Determination of the admissible intervals of the input technological parameters that provide the necessary values of the parameters – acceptance criteria

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Abstract. An inverse optimization problem is considered to determine the optimal intervals of the input technological parameters. The solution is based on multi-response technological process models for the multi-dimensional area of input and output parameters. Expressions for calculating the coefficients of the multi-response models are given. It is shown how the intervals of admissible values of the input technological parameters are built. As an optimality criterion, the percentage of yield of products is used, parameters – acceptance criteria.

1. Parameters - acceptance criteria

The solution of the problem of determining the admissible areas of independent technological (control) parameters \( x_i, i = 1, 2, \ldots, k \) allows rejecting admittedly unsuitable products at the early stages of the technological process and increasing the yield of good products. In practice, there is an area of changes of these parameters, determined by physical causes, which is defined by the system of inequalities in the form \( x_{i1} \leq x_i \leq x_{i2} \). Belonging to the class of acceptability is determined on the basis of output parameters – acceptance criteria, which are measured for the finished products.

The task of determining the permissible areas of the input process parameters is to determine such intervals for the values of the input process parameters that ensure that this product belongs to the class of acceptability at an early stage of the process.

Such a problem is usually solved for the case of a single parameter, the criterion of acceptability [1], which, obviously, limits the applicability of the obtained results so much that they have no practical value. In this paper, the solution of the problem of determining the admissible areas of technological parameters (tolerances) is considered for the case of several output parameters – acceptance criteria, taking into account the multi-response of output parameters.

2. Intervals of the admissible values of output parameters – acceptance criteria

The area of admissible values of output parameters – acceptance criteria \( Y = \{y_1, y_2, \ldots, y_m\}^T \) is represented as a \( m \)-dimensional parallelepiped \( \Omega \) in the space of these parameters. The point \( Y \), representing the finished product in the output parameter area, belongs to this space if its coordinates satisfy the system of inequalities.
where some interval boundaries can be assigned to infinity. Vector $X = \{x_1, x_2, \ldots, x_k\}^T$ is the input controllable technological parameters area which defines a point in the output parameters space, parameters – acceptance criteria $\Omega$ corresponding to this product.

If the transformation is known $X \Rightarrow Y$, then for a given point in the space of input technological parameters it is possible to determine the corresponding point in the space of output parameters – acceptance criteria.

If point $X$ corresponds to point $Y$ inside the space $\Omega$ ($Y \in \Omega$), then this product meets the requirements of technical conditions (TC) for these parameters. Thus, a given $m$-dimensional area $\Omega$ is displayed in the space of input technological parameters in the form of a $k$-dimensional space $\Gamma$ ($m \geq k$).

If image $\Gamma$ of area $\Omega$ is defined, then it gives the possibility to set the technological parameters $X \notin \Gamma$ that provide a priori good products. If the set of parameters – acceptance criteria is determined by the TC, then the composition of the technological parameters $X = \{x_1, x_2, \ldots, x_k\}^T$ is determined using the methods of selection of informative parameters.

Image $\Gamma$ usually has a complex shape. In order to set the input technological parameters independently of each other, you need to set in the area $\Gamma$ a $k$-dimensional parallelepiped $\Pi$, which will determine the independent tolerances on the input technological parameters.

The criterion of optimization $D$ to determine the optimal parallelepiped $\Pi$ may be the yield of good products by technological parameters. This criterion can be expressed as [2]

$$D = \iiint_{\Pi} f(x_1, x_2, \ldots, x_k) dx_1 dx_2 \ldots dx_k,$$

where $\Delta x_i = x_{ih} - x_{il}$ is the maximum length of the interval of variation of the input parameter $x_i$, determined by the TC.

If all input parameters are controllable, then to determine the tolerances of the input parameters, it is necessary to introduce additional restrictions. You can, for example, build area $\Pi$ according to the criterion of the maximum relative width of the intervals of these parameters for a given area of their variations in the form

$$D = \prod_{i=1}^k \frac{x_{ih} - x_{il}}{\Delta x_i},$$

where $f(x_1, x_2, \ldots, x_k)$ is probability density function of the error of technological parameters reproduction, and the point inside $k$-dimensional parallelepiped $\Pi$ is determined by the system of inequalities

$$\begin{align*}
x_{11} &\leq x_1 \leq x_{12} \\
x_{21} &\leq x_2 \leq x_{22} \\
&\vdots \\
x_{k1} &\leq x_k \leq x_{k2}
\end{align*}$$

Figure 1 shows an example of constructing admissible intervals for three input controllable parameters by criterion (2).
Figure 1. Building of admissible intervals of values of input parameters in the form of parallelepiped \( \Pi \) inscribed in the area of admissible values \( \Gamma \) for three input controllable parameters and two output parameters.

3. Multi-response model of the area of admissible values of output parameters

Transformation \( X \Rightarrow Y \) is represented as a multi-response model.

\[
Y = F(X, B) + E, \quad (3)
\]

where \( F(X, B) = \{f_1(X, B), f_2(X, B), \ldots, f_m(X, B)\}^T \) is the \( m \)-dimensional vector of functions, \( X = \{x_1, x_2, \ldots, x_k\}^T \) is the vector of input technological parameters, \( Y = \{y_1, y_2, \ldots, y_m\}^T \) is the vector of output parameters – acceptance criteria, \( B = \{b_1, b_2, \ldots, b_l\}^T \) is the \( l \)-dimensional vector of coefficients, the values of which are to be estimated, \( E = \{e_1, e_2, \ldots, e_m\}^T \) is the observation error of the output parameters (3).

In case of a normal distribution of observational errors \( E \) with zero expectancy and with covariance matrix \( V_E \) for problems of maximum likelihood and pseudo maximum likelihood methods, the objective function for obtaining estimates of coefficients in expression (3) depends on the coefficients through the likelihood function logarithm in [2,3]

\[
\varphi(B) = \sum_{i=1}^{n} [Y_i - F(X_i, B)]V_E^{-1}[Y_i - F(X_i, B)]^T. \quad (4)
\]

where \( n \) is the number of vector \( Y \) observations.

As estimates of coefficients \( \hat{B} \), the values minimizing function (4) are taken. If the model's equations \( Y = F(B, X) \) in the neighborhood of point \( \hat{B} \) can be approximated by equations linear with respect to coefficients in the form

\[
Y = Y^* + \left( P^T(X) \hat{B} \right) (B - \hat{B}), \quad (5)
\]

where

\[
P(X) = \left\{ \frac{\partial f_1(B, X)}{\partial B} \bigg| \hat{B}, \frac{\partial f_2(B, X)}{\partial B} \bigg| \hat{B}, \ldots, \frac{\partial f_m(B, X)}{\partial B} \bigg| \hat{B} \right\},
\]
then the estimates of the coefficients with an unknown covariance matrix $V_E$ can be calculated using the system of equations [4, 5]

$$
\hat{\beta}^{+1} = \hat{\beta}^t + K \sum_{i=1}^{n} P(X_i) S_E^{-1} [Y_i - F(X_i, \hat{\beta}^t)] \\
S_E = \frac{1}{n} \sum_{i=1}^{n} [Y_i - F(X_i, \hat{\beta}^t)] [Y_i - F(X_i, \hat{\beta}^t)]',
$$

where $S_E$ is estimation of covariance matrix $V_E$.

The covariance matrix of coefficient estimates (6) is equal to

$$
K = \left[ \sum_{i=1}^{n} P(X_i) S_E^{-1} P^T(X_i) \right]^{-1}.
$$

As functions $F(X, B) = [f_1(X, B), f_2(X, B), \ldots, f_m(X, B)]^T$ for modeling technological processes, quadratic polynomials with all interactions are usually used. In this case, function $P(X)$ in the expression (5) takes the form

$$
P^T(X) = \begin{bmatrix}
1, x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1 x_2, x_1 x_3, \ldots, x_{k-1} x_k \\
1, x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1 x_2, x_1 x_3, \ldots, x_{k-1} x_k \\
\ldots \\
1, x_1, x_2, \ldots, x_k, x_1^2, x_2^2, \ldots, x_k^2, x_1 x_2, x_1 x_3, \ldots, x_{k-1} x_k
\end{bmatrix}.
$$

Then, step regression procedure is applied to this model with decrease in the number of members. In the step regression procedure, the coefficients are found for which the inequality holds

$$
\frac{f_i}{\sqrt{k_i}} \leq t_{1-\alpha, 2},
$$

where $k_i$ is the diagonal element of matrix $K$ for the $i$-th coefficient, $t_{1-\alpha, 2}$ is the quantile of the Student's distribution at the significance level $\alpha$.

Members that include coefficients that satisfy inequality (8) are excluded from the corresponding functions, and the estimates of the coefficients are recalculated and the procedure for reducing the number of members of the model is repeated.

4. Determining the image of the area of acceptable values of output parameters

After performing the step regression, clarifying the type of functions $f_1(X, B), f_2(X, B), \ldots, f_m(X, B)$ and determining the estimates of all significant coefficients of model (2), expression $Y = F(\hat{\beta}, X)$ allows us to build area $\Gamma$. In some rare practical situations this area can be built analytically. Generally, the principle of building of this area consists in determining the projections of this area on separate planes of the projections of the space of technological parameters and building for each of these projections an inscribed rectangle that represents the projection of area of admissible values $\Pi$ on this plane.

Consider the process of building area $\Gamma$ on the illustrative example of a two-response function with two technological parameters in the form

$$
F(X, B) = \begin{bmatrix}
y_1 = b_7 + b_6 x_1 + b_5 x_2 + b_4 x_1^2 + b_3 x_1 x_2 + b_2 x_2^2 \\
y_2 = b_7 + b_6 x_1 + b_5 x_2 + b_4 x_1^2 + b_3 x_1 x_2 + b_2 x_2^2
\end{bmatrix}.
$$

For specified intervals of valid values of parameters – acceptance criteria in the form

$$
\frac{f_i}{\sqrt{k_i}} \leq t_{1-\alpha, 2},
$$

where $k_i$ is the diagonal element of matrix $K$ for the $i$-th coefficient, $t_{1-\alpha, 2}$ is the quantile of the Student's distribution at the significance level $\alpha$. Members that include coefficients that satisfy inequality (8) are excluded from the corresponding functions, and the estimates of the coefficients are recalculated and the procedure for reducing the number of members of the model is repeated.
\[
\begin{cases}
y_{11} \leq y_1 \leq y_{12} \\
y_{21} \leq y_2 \leq y_{22}
\end{cases}
\]

In the space of technological parameters \(x_1, x_2\), it is possible to obtain two areas of admissible values: for parameter \(y_1\) – area \(\Gamma_1\), and for parameter \(y_2\) – area \(\Gamma_2\). The joint area of admissible values of technological parameters \(\Gamma\) is defined as \(\Gamma = \Gamma_1 \cup \Gamma_2\) (figure 2).

To build area \(\Gamma\) with a confidence probability \(P\), as model \(Y = F(\hat{\theta}, X)\) coefficient values the corresponding one-sided boundaries of their confidence intervals are used as the values of the coefficients of the model (to obtain the minimum area) in the form

\[b_i \leq \hat{\theta}_i \pm \sqrt{t_{1-\alpha} s_i},\]

where \(P = 1 - \alpha\), \(i = 1, 2, \ldots l\).

**Figure 2.** Obtaining the joint area of admissible values of technological parameters for a two-response quadratic function: \(\Gamma_1\) is the area of admissible values for parameter \(y_1\), \(\Gamma_2\) is the area of admissible values for parameter \(y_2\), \(\Gamma = \Gamma_1 \cup \Gamma_2\).

5. **Calculation of intervals of admissible values of technological parameters**

To obtain independent intervals of admissible values of technological parameters, a \(k\)-dimensional parallelepiped must be inserted in area \(\Gamma\) in accordance with the optimality criterion (1), which represents the yield of the product under given technological tolerances. Figure 3 shows an illustration of a two-dimensional problem (9) with quadratic functions \(Y = F(\hat{\theta}, X)\).
Figure 3. Building of rectangular area \( \Pi \) of admissible values of technological parameters for two-dimensional quadratic function \( F(\mathbf{b}, \mathbf{x}) \), \( f_1(x) \) and \( f_2(x) \) are distribution density of technological parameters \( x_1 \) and \( x_2 \) respectively.

If, along with uncontrolled input parameters, there are also controlled technical parameters, then optimization by criterion (3) makes it possible to determine the values of these parameters that provide the highest yield. Figure 4 shows the example of determining the optimal tolerances for input uncontrolled parameters \( x_1 \) and \( x_2 \) with distribution densities \( \varphi_1 \) and \( \varphi_2 \), and the optimal value \( x_{30} \) of the controlled input parameter \( x_3 \) providing the highest yield by criterion (3).

![Diagram showing the building of admissible intervals and the determination of optimal tolerances for input parameters](image)

Figure 4. Determination of the admissible intervals for two uncontrolled input parameters and the optimal value of one controlled input parameter for the two-response model.

The use of the optimality criterion (2) makes it possible to build admissible intervals of input parameters, which provide the most convenient control of technological process, when there is no need to ensure the exact values of input parameters.
Due to the large dimension of the input parameters space and the complex shape of the area of admissible values of the parameters – acceptance criteria in the multicriteria case, the solution of optimal problems by criteria (2) and (3) is performed by the Monte Carlo method.

Figure 3 shows that with proper adjustment of the technological process by shifting the centers of the distribution of the input technological parameters, even with a constant variation of these parameters, it is possible to increase the yield. This allows, also, determining the maximum value of the variation of the input technological parameters to ensure the required percentage of yield. When statistically independent errors of observation of technological parameters and optimization criterion (1) takes the following form:

\[ D = \int_{x_{11}}^{x_{22}} f_1(x) dx \int_{x_{11}}^{x_{22}} f_2(x) dx. \]

The building of area \( \Pi \) is carried out by statistical modeling method.

6. Conclusion
The proposed method of determining technological tolerances allows determining independent intervals of admissible values of technological parameters, which makes it possible to reject unsuitable products in the technological process to ensure the necessary values of parameters – acceptance criteria of finished products. This method, in addition, makes it possible to work out recommendations on how to adjust the technological process in order to increase the yield, both by optimizing the position of the distribution centers of the technological parameters and in relation to their spread.

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