Optimal experimental design for multi-response modeling of technological processes

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Abstract. The problem of optimal experimental design for the construction of multi-response models of the technological process is considered. Optimal experimental design can significantly improve the accuracy of model building and their predictive ability.

1. Introduction

The location of observation points of input parameters \( X_i, \ i = 1, n \), \( n \) is the number of observations in the region of experiment planning of the technological process in the space of input parameters, determines the accuracy of estimating the coefficients of the model, which connect input and output parameters, and the accuracy of prediction of response by the model type [1]

\[
Y = F(B, X) + E, \quad (1)
\]

where \( Y \) is the vector of output parameters, \( F \) is the multi-response function of the vector of input parameters \( X \) and the vector of coefficients \( B \), \( E \) is the vector of observation errors of the output parameters.

Practically all production tasks of the modeling of technological processes are of multi-response nature and the experimental designs are built for the multi-response space of output parameters. If the observation points are arranged in the space of input parameters in accordance with the optimal experiment design, then the prediction accuracy according to model (1) will be the maximal with the same number of observations. The design of experiments \( \Delta \), thus, is a set of observation points \( \{X_1, X_2, ..., X_n\} \) in the space of the input parameters of the technological process.

2. Prediction by the model

Prediction of the future values of output parameters (responses) is the main goal of building a mathematical model. These values provide estimates of the coefficients of the model (1), which determine the prediction equations. If the model used is correct (adequate), then there are two possible sources of inaccuracy in the predictions: errors in the estimates of the \( B \) coefficients and errors in the observations of the response vector. These two sources contribute to the differences between the predicted and actually observed response values.

It is usually assumed that the errors generated by these sources are statistically independent. Then it is possible to calculate the covariance matrix of prediction errors. The observed value of the vector \( Y \) will be determined by the formula

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

where \( \delta B \) is the estimation errors of the model coefficients.
Decomposition of a Taylor series, limited to only linear terms, leads to equality
\[ \delta Y = \frac{\partial F}{\partial B} \delta B + E. \]

Then the covariance matrix of response estimates is represented by expression (2)
\[ V_{y} = P(\hat{B}, X)^{T} V_{B} P(\hat{B}, X) + V_{E}, \] (2)
where \( P(B, X) = \left\{ \frac{\partial f_{1}(B, X)}{\partial B}, \frac{\partial f_{2}(B, X)}{\partial B}, \ldots, \frac{\partial f_{m}(B, X)}{\partial B} \right\} \), \( B \) is the model coefficient estimates (1), \( V_{B} \) is the coefficients covariance matrix and \( V_{E} \) is the errors covariance matrix.

Optimal experimental design allows you to increase the accuracy of estimation of the coefficients of the model. The covariance matrix of observation errors \( V_{E} \) is assumed constant, therefore the quality of the model prediction is estimated by the value of the covariance matrix of the average prediction error \( V_{Y} \) in the center of the design area without taking into account matrix \( V_{E} \) as
\[ V_{y} = P(\hat{B}, X)^{T} V_{B} P(\hat{B}, X). \] (3)

Thus, as a criterion for the optimality of the design in this case, you can take the determinant of the covariance matrix \( \det V_{Y} \). To calculate this optimality criterion, it is necessary for a given experimental design to calculate the covariance matrix of the coefficient estimates, and then, using formula (3), calculate the covariance matrix of the response estimates in the center of the design area and its determinant. The optimal designs obtained for this criterion of optimality are called \( G \)-optimal. It is known that the continuous \( G \)-optimal designs, instead of the optimality criterion in the form of \( \det V_{Y} \), one can use the optimality criterion in the form of \( \det V_{B} \). This greatly increases the accuracy of the coefficients calculation and speeds up the design process, as it simplifies the calculation of the optimality criterion.

Optimal designs that use the value of \( \det V_{B} \) as a criterion for optimality are called \( D \)-optimal.

3. \( D \)-optimal design of experiments

The criterion of \( D \)-optimality requires such an arrangement of experimental points in the design area of the experiment \( \Sigma \), in which the determinant \( \det V_{B} \) of matrix \( V_{B} \) is minimal. The \( D \)-optimal design minimizes the amount of ellipsoid of scattering coefficient estimates in the form of [2]
\[ D = \det V_{B}. \] (4)

Thus, the \( D \)-optimal design is defined as follows:
\[ \det V_{p}(\Delta) = \min_{\Delta \subseteq \Sigma} \det \left\{ \sum_{j=1}^{n} P(\hat{B}, X_{j}) V_{E}^{-1} P(\hat{B}, X_{j})^{T} \right\} = \max_{\Delta \subseteq \Sigma} \det \left\{ \sum_{j=1}^{n} (\hat{B}, X_{j}) V_{E}^{-1} P(\hat{B}, X_{j})^{T} \right\}, \] (5)
where \( \Delta = \left( X_{1}^{0}, X_{2}^{0}, \ldots, X_{l}^{0}, \ldots, X_{n}^{0} \right) \) is the optimal design in the sense of the \( D \)-optimality criterion.

There are discrete \( D \)-optimal designs, which are built for a predetermined number of experiment points, and continuous \( D \)-optimal designs, the number of points of which significantly exceeds the number of model coefficients. Continuous designs are characterized by a finite spectrum and frequency of experiment points at each point of the design spectrum.

The number of points \( r \) of the spectrum of continuous \( D \)-optimal designs satisfy the following inequality [3]
\[ l + 1 \leq r \leq \frac{(l+1)(l+2)}{2}, \]
where \( l \) is the number of estimated coefficients of model (1).

It is known that the continuous \( D \)-optimal designs coincide with the \( G \)-optimal designs. In this case, it is easier to build the \( D \)-optimal designs, while the resulting design will also be \( G \)-optimal. The analytical way of constructing continuous \( D \)-optimal designs and their subsequent rounding to discrete designs is used to obtain designs only in the simplest cases. In practice, there are a large number of tasks in which the design area \( \Sigma_{X} \) does not have a regular geometric shape, and the model is presented in a rather complicated way, for example, in the form of a computer program. In these cases, to build optimal
designs, it is necessary to use numerical methods associated with minimizing the determinant \( \det V_B \) of the covariance matrix of coefficient estimates \[3\].

Extremum problem (5) has the dimension of \( mn \), where \( n \) is the number of points of the experiment design, \( m \) is the number of observed output parameters and is complex in the sense of convergence of the computational procedure and computer time spent using standard extremum search procedures.

4. Building multi-response sequential designs

A priori experimental designs, which are constructed prior to the experiment, can only be constructed for linear single-response models. For nonlinear models, the use of a priori experimental designs is based on an average result and usually does not provide the necessary accuracy of estimating the output parameters for a particular product situation. Often, as a condition to stop the construction of an optimal design, the accuracy of estimating the coefficient estimates is set. This condition determines the number of points in the design. However, even for a large number of observation points of an a priori design for a specific task, the accuracy of estimation is much worse than required. This is due to the fact that the optimal design is built for the average values of the parameters, and the actual values of the output parameters can often differ significantly. The use of such design is justified when the design needs to be built prior to the experiment, for example, due to technical limitations imposed on the technological process.

More efficient is the sequential planning procedure. In this case, some initial design of the experiment is set up with a relatively small number of observation points \( n \). As such a design, you can use, for example, a uniform experimental design that uniformly covers the entire design area.

Using this design, experiments are performed and estimates of the coefficients of the model are calculated. Based on the estimates obtained, the next \((n + 1)\)-th observation point is found, adding which to the experimental design ensures the best estimation accuracy. The number of observations increases until the required actual accuracy of estimating the output parameters for this model is achieved.

The algorithm for building sequential design can be represented by the following expression \[4\].

\[
det V_B(\Delta + X^0, B) = \min_{X \in \Sigma} \det V_B(\Delta + X, B)
\]  

(6)

where \( X^0 \) is the point added to design \( \Delta \).

The accuracy of estimating the output parameters in the center of the design area is calculated as follows.

\[
V_y = P(\hat{B}, X)^T V_B P(\hat{B}, X),
\]

(7)

where \( X \) is the input parameter vector in the center of the experiment design.

To perform the search for extremum, in accordance with the expression (6), the initial design of the experiment is set. The initial design is generated using a random number generator for a given number of experiment points and for a given area of the independent input parameters.

The search for the optimal design is carried out several times for various generated initial design generated by computer. The design that provides the smallest determinant of the covariance matrix for estimating the coefficients of the model (5) is taken as the optimal experimental design. Usually it takes no more than 20-50 iterations to find the global extremum using formulas (6,7).

5. Algorithm for building \( D \)-optimal design using the half-division method

After specifying the initial design, the optimal design is searched for in accordance with the above mentioned algorithm using the half-division method. A penalty function is also introduced to ensure the search for an extremum in a given area of variation of the parameters. The search algorithm is as follows [5].

1. The number of control points \( n \) is set and an arbitrary initial experiment design is determined. \( \Delta^1 = \{X^1_1, X^1_2, ..., X^1_m\} \).
2. The first control point is selected to search for a particular extreme \( X_i \).
3. Separately, for each parameter, the partial search method solves a particular extremal problem for one variable of the control point \( X_i \) and for the rest of the fixed points \( X_1, X_2, ..., X_i, ..., X_n \). Trial steps
are performed and a step is taken in the direction of decreasing the objective function. If the specified parameter is outside the specified limits of its variation, then the value of the objective function is given by the introduction of a penalty.

If in both directions the objective function increases, then the length of the trial step is reduced by half. As the stop criterion the search step length, which determines the accuracy of the input parameters, is taken.

The search is repeated for all parameters and this point of the plan. The resulting point is added to the design \( \Delta_1 = (X^1_1, X^2_1, ..., X^i_1, ..., X^n_1) \) instead of the starting point. Thus, a design \( \Delta_2 = \Delta_1 - X^1_{i1} + X^2_{i1} \) is defined in the form

\[
\Delta_2 = (X^1_1, X^2_1, ..., X^i_1, ..., X^n_1),
\]

where the point is defined as follows:

\[
det\{V_B(\Delta^1 - X^1_{i1} + X^2_{i1}, B)\} = \min_{X \in \Sigma} \det\{V_B(\Delta^1 - X^1_{i1} + X, B)\}
\] (8)

1. The search is repeated for all points of the initial design.
2. The criterion for stopping the entire procedure is the relative variation in the objective function.

If this criterion is not met, the search procedure 2–4 is repeated.

For example, an optimal design is obtained for 14 points with a single covariance matrix of observation errors and a two-response quadratic model with two responses (output parameters) with 12 coefficients, the form of which is represented as follows:

\[
y^1 = b_1 + b_{23}x_3 + b_{41}x_1x_1 + b_{5}x_1 + b_{6}x_2x_2
\]

\[
y^2 = b_7 + b_{8}x_1 + b_{9}x_2 + b_{10}x_1x_1 + b_{11}x_1x_1 + b_{12}x_2x_2
\] (9)

Figure 1 shows the initial design for 14 points of the experiment. As an optimality, the expression is taken \( D' = D^{-1} = -\log(\det V^*_b) \) for which increase means decrease in the covariance matrix \( \det V^*_b \).

![Figure 1](image1.jpg) Figure 1. The experimental design for 14 points, obtained using a random number generator and used as an initial approximation for model (9). The marked points show the experimental design. \( D' = 22.789 \).

Figure 2 shows the optimal design, obtained on the basis of algorithm (8).

![Figure 2](image2.jpg) Figure 2. The experimental design obtained after optimization by the search method. Larger circles marked points of the design, including two observations. \( D' = 25.109 \). Such design exactly corresponds to the theoretical one.

For model (9) for 12 design points, an optimal experiment design was constructed in the sense of criterion (6) with uniform probability distributions of coefficients. Thus, as an optimality criterion in this case, for a model that is nonlinear in terms of coefficients, the average determinant of the covariance matrix of coefficient estimates was taken as
\[
\overline{\text{det}} V_B(\Delta^0) = \min_{\Pi \in \Sigma} \overline{\text{det}} V_B(\Delta). \tag{10}
\]

When calculating, the admissible ranges of values for each of the model coefficients were specified in the form of a lower bound and the length of the coefficient variation with a diagonal unity covariance matrix of observation errors.

The number of statistical tests was 10,000. As an initial design, uniform design for 12 points was used. For this design and non-linear model, the average determinant \(\overline{\text{det}} V_B(\Delta)\) of the covariance matrix \(V_B\) of the coefficients is \(= 28.607\).

Figure 3 shows the experimental design obtained by the half division method for uniform a priori probability distributions of the coefficients.

![Figure 3](image1.png)

**Figure 3.** The optimal experiment design obtained by the search method for 12 points. \(D' = 28.785\).

Figure 4 shows experimental design built for the case when all coefficients are known. \(D' = 28.785\).

![Figure 4](image2.png)

**Figure 4.** The experimental design for 12 points, obtained with the known coefficients of the model. Large circles marked points of the design, including two observations. \(D' = 31.800\).

### 6. The sequential algorithm of design building

The sequential design program is implemented in accordance with expression (6) and is based on all the programs described earlier: obtaining an initial uniform design, calculating estimates of the coefficients of a non-linear model with an unknown observational error covariance matrix, calculating the coefficient of the covariance matrix of estimating coefficients, and finding the optimal design point using the half division.

1. The initial design of the experiment is set \(\Pi^I (s = 0)\) such and with so many points \(n\) that the information matrix is sufficiently well defined.

2. In accordance with this design, measurements of technical parameters are performed, estimates of the coefficients of the model and the criterion of optimality of the design (10) are calculated.

3. To the design is added another point in the middle of the area of variation of the measured parameters.
4. The search method searches for the \((n + s)\) -th point of the experiment \(s = s + 1\) \(X_{n+s}\) such that adding this point to the existing experiment design \(\Pi_{s+1} = \Pi_s + X_{n+s}\) provides the maximum increase in the estimation accuracy, i.e.,

\[
\det[V_B(\Pi^s + X^0_{n+s}, B)] = \min_{U \in U} \det[V_B(\Pi^s + X_{n+s}, B)].
\]  

(11)

5. Observation is performed at the obtained point of the design. The stop criterion is the specified limit value of the determinant of the covariance matrix.

6. If this criterion is not met, the next point is added to the design.

The procedure of sequential designing allows to obtain the accuracy of determining the coefficients of the model not worse than the specified one.

Table 1 shows the \(D\)-optimality criteria in the form of a quantity \(D'\) calculated for various types of experimental designs for the model in the form of two-dimensional polynomial (9).

| Number of points | Uniform with given coefficients | Optimal for given coefficients | Uniform for given probability distribution of coefficients | Optimal for given probability distribution of coefficients | Sequential experimental design |
|------------------|---------------------------------|-------------------------------|--------------------------------------------------------|--------------------------------------------------------|-------------------------------|
| 12               | 31.031                          | 30.338                        | 28.607                                                 | 28.785                                                 | 31.162                        |
| 20               | 32.583                          | 33.553                        | 29.246                                                 | 29.493                                                 | 33.268                        |
| 50               | 35.274                          | 34.671                        | 41.959                                                 | 32.241                                                 | 36.128                        |
| 100              | 37.05                           | 39.120                        | 34.587                                                 | 35.744                                                 | 38.757                        |

7. Conclusion
The modeling of technological processes in the form of multi-response models is a necessary condition for obtaining adequate models. The use of optimal multi-variant experimental designs by several orders of magnitude improves the accuracy of estimating the coefficients of a multi-response model. The specific examples show how to construct a priori and sequential experiment design.

The use of the procedure of sequential design reduces the determinant of the covariance matrix of the coefficient estimates in comparison with the a priori optimal design built for a given probability distribution of coefficients by 2–4 times.

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