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Mathematical modeling of compositional rotatable plans in problems of mechanics

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Abstract: The article proposes a methodology for conducting tests using the theory of experiment planning. The elements of regression analysis are detailed. The results on multiple regression are presented, the basic provisions of the theory of planning of experiment are presented, planning criteria are discussed. The possibility of reducing the number of experiments by conducting a fractional factorial experiment is discussed. Box and Hartley composite plans and rotatable, centered composite plans are presented.

Key words: Experiment planning, Replica, Factor, Trials, Composition, Plan, Equation, Observations

1. Introduction

The main feature of all methods of the theory of planning of experiment (TPE), as it is nown, is a multifactorial approach to conducting an experiment, providing not alternate, but simultaneous change from point to point of all acting factors [1-3]. The methods of drawing up optimal plans of multifactor experiment developed in the theory allow to choose the most informative combinations of values of determining factors for conducting experiments and reasonably assign the number of experiments necessary and sufficient to obtain the result with the required completeness and accuracy [4-7].

The results of the experiments conducted in accordance with the multivariate plan are processed so as to determine the coefficients of the regression equation of a pre-selected type (usually polynomial) using the measured values and, thus, to obtain a mathematical description of the dependence of the studied parameters or characteristics of the object (response functions) on the determining factors and their interactions [5].

2. The structure of the central compositional plans

The plan to which corresponds the response function

$$\eta = \beta_0 + \sum_{1 \le i \le k} \beta_i x_i + \sum_{1 \le i_1 < i_2 \le k} \beta_{i_1 i_2} x_{i_1} x_{i_2} + ... + \sum_{\substack{i_1, \ldots, i_k \\ \sum i_j = d}} \beta_{i_1 \ldots i_k} x_1^{i_1} ... x_k^{i_k} \qquad (1)$$

which is a polynomial of degree d from the variables $x_1, x_2, \ldots, x_k$, is called a plan of order d if it allows us to obtain unbiased (separate) least squares method of estimating unknown response parameters $\beta_0, \{\beta_i\}, \{\beta_{i_1 i_2}\}, ..., \{\beta_{i_1 ... i_k}\}$. The number of unknown parameters in (1.1) is C^d_{k+d}.

A polynomial of degree 2 is usually used to approximate the region of extremum

$$\eta = \beta_0 + \sum_{1 \le i \le k} \beta_i x_i + \sum_{1 \le i < j \le k} \beta_{ij} x_i x_j + \sum_{1 \le i \le k} \beta_{ii} x_i^2 \quad (2)$$

When approximating the extremum region by a second-order hypersurface, the problem of choosing an experiment plan arises. To construct second-order plans, we cannot directly use factor experiments in which the variables are varied at two levels. These experiments do not allow us to obtain separate estimates of the parameters $\beta_0, \{\beta_{ii}\}$, because for them $x_1^2 = x_2^2 = ... = x_k^2 = 1$. Therefore, factor experiments in which variables are varied at three or more levels are used to construct second-order plans. In the central composite plans, the variables vary at five levels.

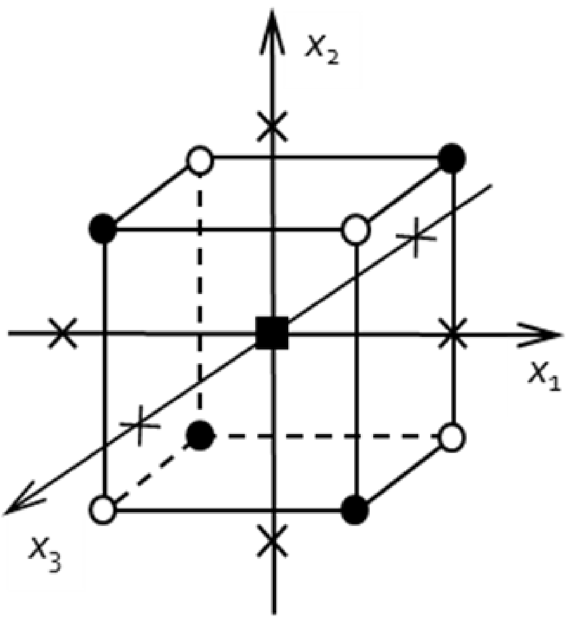

Figure 1: Geometric reflection of the full factorial experiment plan of type 2^3 in the factor space.

2.1. Methodology for building plans

Let us consider an example of building a central compositional plan when the number of factors $k = 3$. Full factorial experiment (FFE) 2^3 forms the core of the compositional plan (in Fig. 1 the core of the plan is depicted by circles and blackened points). As additional points for observations, we take six more so-called "star" points with coordinates $(-\alpha_1, 0, 0)$, $(\alpha_1, 0, 0)$, $(0, -\alpha_2, 0)$, $(0, \alpha_2, 0)$, $(0, 0, -\alpha_3)$, $(0, 0, \alpha_3)$ (marked with crosses in Figure 1). In addition to the above points, n0 parallel (repeated) experiments in its center (blackened square in Figure 1) are used when constructing the compositional plan. They are necessary to test the hypothesis of model adequacy and to obtain information about the center of the plan. The plan matrix (Figure 1) at has $n_0 = 2$ the form

$$\overline{D} = \begin{pmatrix} \overline{D}_1 \\ \overline{D}_2 \end{pmatrix}, \quad \text{where } \overline{D}_1 = \begin{pmatrix} - & - & - \\ + & - & - \\ - & + & - \\ + & + & - \\ - & - & + \\ + & - & + \\ - & + & + \\ + & + & + \end{pmatrix}, \quad \overline{D}_2 = \begin{pmatrix} -\alpha_1 & 0 & 0 \\ \alpha_1 & 0 & 0 \\ 0 & -\alpha_2 & 0 \\ 0 & \alpha_2 & 0 \\ 0 & 0 & -\alpha_3 \\ 0 & 0 & \alpha_3 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

The plan is a composition or connection of two plans and is therefore called a compositional plan. Since the points of the constructed composite plan are symmetrically located relative to the center, it is called a central plan.In the considered plan the number of experiments $N = 2^3+2*3+2 = 16$, and in the FFE $N = 27$. Similarly, the second-order central composite plans are constructed for any number of factors k, with each of the factors x_i varying at five levels: $-\alpha_i$, -1, 0, α_i, 1 $(i = 1, 2, ..., k)$. A second-order central compositional plan (CCP) is obtained by completing a two-level factor plan of type $2^{k-q}(0 \le q < k)$ by joining star and center points to it. The factor plan of type in this case is called the core of the plan.
The second-order matrix of the CCP is as follows $[8-10]$:

$$\overline{D} = \begin{pmatrix} \overline{D}_1 \\ \overline{D}_2 \end{pmatrix}$$

where $\overline{D}_1$the matrix of the factor plan;

$$\overline{D}_2 = \begin{pmatrix} -\alpha_1 & 0 & ... & 0 \\ \alpha_1 & 0 & ... & 0 \\ 0 & -\alpha_2 & ... & 0 \\ 0 & \alpha_2 & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & 0 & -\alpha_k \\ 0 & 0 & 0 & \alpha_k \\ 0 & 0 & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & ... & 0 \end{pmatrix}$$

- is the matrix of the “star” plan. The matrix $\overline{D}_2$ has order $(2k + n_0)k$. The number of observations $N = N_0 + 2k + n_0$,

where N_0-is the number of observations at the core points of the plan; $2k$ is the number of “star” points; is the number of observations at the center of the plan. The number of different points of the plan, respectively $N^* = 2^{k-q} + 2k + 1$.

Next, we consider plans for which $\alpha_i = \alpha(i = 1, 2, ..., k)$. All points of such plans are located on three hyperspheres, one of which is degenerate. A necessary condition for the existence of unbiased least squares estimates $p + 1$ of the unknown coefficients in equation (3.2) when a regular fractional replica is chosen as the plan kernel is the condition $p+1 \le N^*$. When $q = 0$, this condition is sufficient for any $k \ge 2$.

Table 2.1 shows the matrix of independent variables of the second-order CCP. Plus and minus signs mean that variables $x_1, x_2, ..., x_k$ and their pairwise interactions take values either positive or negative.

Table 1: Central compositional plan (CCP)

Plan	Number of observations	Matrix of independent variables X		
		$x_0\ x_1\ x_2 \dots x_k$	$x_1 x_2 \dots x_{k-1} x_k$	$x_1^2\ x_2^2 \dots x_k^2$
fractional factor experiment (FrFE) 2^{k-q}	2^{k-q}	$1\ \pm1\ \pm1 \dots \pm1$	$\pm1 \dots \pm1$	$1\ 1 \dots 1$
		$1\ \pm1\ \pm1 \dots \pm1$	$\pm1 \dots \pm1$	$1\ 1 \dots 1$
		$\dots\dots\dots$	$\dots\dots$	$\dots\dots\dots$
		$1\ \pm1\ \pm1 \dots \pm1$	$\pm1 \dots \pm1$	$1\ 1 \dots 1$
«star»	$2k$	$1\ -\alpha\ 0 \dots 0$	$0 \dots 0$	$\alpha^2\ 0 \dots 0$
		$1\ \alpha\ 0 \dots 0$	$0 \dots 0$	$\alpha^2\ 0 \dots 0$
		$1\ 0\ -\alpha \dots 0$	$0 \dots 0$	$0\ \alpha^2 \dots 0$
		$1\ 0\ \alpha \dots 0$	$0 \dots 0$	$0\ \alpha^2 \dots 0$
		$\dots\dots\dots$	$\dots\dots$	$\dots\dots\dots$
		$1\ 0\ 0 \dots -\alpha$	$0 \dots 0$	$0\ 0 \dots \alpha^2$
		$1\ 0\ 0 \dots \alpha$	$0 \dots 0$	$0\ 0 \dots \alpha^2$
Observations in the center of the plan	n_0	$1\ 0\ 0 \dots 0$	$0 \dots 0$	$0\ 0 \dots 0$
		$\dots\dots\dots$	$\dots\dots$	$\dots\dots\dots$
		$1\ 0\ 0 \dots 0$	$0 \dots 0$	$0\ 0 \dots 0$

The fractional replica used as the core of the CCP must satisfy certain requirements. Otherwise, the CCP will not allow to obtain unbiased least squares method estimates of unknown coefficients, i.e. it will not be a second-order plan.
A fractional replica of type 2^{k-q} can be a second-order CCP kernel if and only if any two pairwise interactions for this replica are modulo not equal to each other, i.e., when

$$x_i x_j \neq \pm x_l x_s;\ i, j, l, s = 1, 2, ..., k;\ i \neq j,\ l \neq s,\ (i, j) \neq (l, s) \quad (3)$$

order.
Let us show that. A CCP will be a second-order plan if and only if the matrix of independent variables corresponding to a polynomial of degree 2 has maximal rank. Let some pairwise interactions in the plan kernel be modulo equal, i.e., condition (3) is violated. Then the columns of the matrix of independent variables corresponding to these interactions will also be equal without taking into account the sign and, therefore, linearly dependent. Let now condition (3) be satisfied. Then no column of the matrix of independent variables can be represented as a linear combination of its other columns and, therefore, its rank will be maximal.

We can conclude that by the construction of the 2nd-order CCP, any two pairwise interactions at the points of the plan kernel are modulo not equal, i.e., condition (3) is satisfied.

The main feature of the CCPs is that they allow us to apply methods of sequential planning of the experiment. First, a fractional factor experiment (FrFE) of type 2^{k-q} is constructed to analyze the response surface. Then, if the results of the analysis do not satisfy the researcher, the FrFE is completed to the CCP and a more complete study of the response surface is carried out. In this case, composite plans give a gain in the number of experiments compared to other plans. These plans can be applied also at direct construction of response function in the form of polynomial (2).

2.2. Box plans

Among the CCP , Box plans are the most widely used due to some of their valuable properties. A second-order CCP is called a Boxing plan if its core is a 2^k FFE or a regular replica of type 2^{k-q} for which pairwise interactions are not modulo linear variables, i.e.

$$x_i \neq \pm x_j x_l;\ i, j, l, = 1, 2, ..., k;\ j \neq l. \quad (4)$$

To construct a Box plans when the core is a fractional replica of 2^k, we use q generating relations, which must be specified using variables $x_1, x_2, ..., x_k$, where $r = k - q$. It follows immediately from (2.3) and (2.4) that generating relations of the form
$x_l = \pm x_i x_j x_l,\ r+1 \leq l \leq k;\ 1 \leq i < j \leq r;\ x_s = \pm x_i x_j x_l + 1 \leq s \leq k;\ 1 \leq i < j < l \leq r;$ or defining contrasts
$1 = \pm x_i x_j x_l, 1 \leq i < j \leq r; r+1 \leq l \leq k; 1 = \pm x_i x_j x_l x_s, 1 \leq i < j < l <\leq r; r+1 \leq s \leq k.$

Thus, the resolving power of the fractional replica 2^{k-q} must be greater than four. A CCP will be a Box plan if the fractional replica 2^{k-q} , which enters it as a kernel, has a resolution greater than or equal to five. Thus, the problem of constructing a Box plan reduces to the problem of constructing regular replicas with resolution greater than or equal to five.

Consequently, at $k < 5$ the core of the Box plan is only the FFE 2^k , and at $k \geq 5$ it can be a half-replica, a quarter-replica, etc. At $2k = 5$ the core of the Box plan besides the FFE 2^5 can be a half-replica 2_v^{5-1}, defined, for example, by the generating relation $x_5 = x_1 x_2 x_3 x_4$ or the defining contrast $1 = x_1 x_2 x_3 x_4 x_5$. The pairwise interactions for this replica are equal to triples and hence conditions (3) and (4) are satisfied. Another Box plan can be constructed using as a kernel a half-replica with defining contrast $1 = -x_1 x_2 x_3 x_4 x_5$.

Let $B_k(N_0 s)$ – be a Box plan for a fixed number of variables k whose kernel contains $(N_0 s)$ different points. Let $B_k = B + k(N_0 s)(s = 1, 2, ..., S)$ be the set of all Box plans for a given k. A Box plan $B_k(N_0)$ is called minimal if $N_0 = \min N_0 1, N_0 2, ..., N_0 s$. Thus, when , Box plans using half-replicates as kernel , will be minimal. The number of experiments in such a plan at is , and in FFE – . The task of constructing minimal plans at large values of turns out to be the most difficult. Depending on the choice of the value of , the Box plan can be made either orthogonal or rotatable. It is impossible to make it both orthogonal and rotatable.

2.3. Hartley plans

It is often necessary to use plans with a small redundancy of experiments. Hartley plans are among such plans in the class of CCP. A second-order CCP is called a Hartley plan if a regular fractional replica from a FFE of type 2^k, in which some pairwise interactions are modulo linear variables, is used as its kernel. That is, condition (3) is satisfied for the Hartley plan, but condition (4) is violated.

Thus, an arbitrary second-order CCP will be either a Box plan or a Hartley plan. Let C_k be the set of second-order CCPs for a fixed number of variables k , and let $H_k = H_k(N_0 t)(t = 1, 2, ..., T)$ be its subset of Hartley plans. Here $N_0 t$ is the number of points in the core of the plan $H_k(N_0 t)$. Then $C_k = H_k B_k; H_k \cap B_k = \phi$.

The greatest practical sense has the application of Hartley minimum plans. The notion of Hartley minimum plan is introduced similarly to the notion of Box minimum plan.

A Hartley plan is called minimal if it requires the smallest possible number of experiments for a given number of factors. According to the definition of the Hartley plan, only fractional replicas with resolution equal to III, i.e., of type 2_{III}^{k-p} can be used to construct its kernel. These replicas must satisfy the condition (3). The plan corresponds to the kernel of 2_{III}^{k-p}, where $p = \lfloor \frac{k}{2} \rfloor$. Thus, constructing a minimal Hartley plan for a given k is equivalent to the problem of finding $2_{III}^{k - \lfloor \frac{k}{2} \rfloor}$.

Let us construct a Hartley plan for $k = 5$ and $m = 2$. As a kernel we take a type $2_{III}^{5-2} = 2_{III}^3$ semireplica with generating relation $I = X_1 X_2 X_4 = X_1 X_3 X_5$. The system of equalities for pairwise interactions for it has the form $X_1 X_2 = X_4 X_5$; $X_1 X_3 = X_4 X_5$; $X_1 X_4 = X_2 X_5$; $X_1 X_5 = X_2 X_4$; $X_2 X_3 = X_3 X_4$; $X_3 X_5 = X_2 X_4$.

The pairwise interactions are not equal to each other, and it itself has a resolution of III.

The number of experiments in this plan is $2^{5-2} = 2^3 = 8$. The plan is minimal because the 2^{5-3} fractional replica cannot be used as the core.

Let us construct the kernel of the Hartley plan for $k = 4$. The kernel of the plan can be a half-replica 2^{4-1}_{III} with generating relation $I = X_1X_2X_3X_4$. The half-replica has a resolution equal to III and pairwise interactions in it are uncorrelated. The plan will be minimal.

Indeed, for fractional replicas of 2^{4-2}, some pairwise interactions are modulo each other. Let replica be given by the defining contrasts $I = X_1X_2X_3$ and $I = X_1X_2X_4$. Then the generalized defining contrast is of the form $I = X_3X_4$. It follows that the pairwise interactions of X_3 and X_4 are equal.

Similarly, it can be shown that for the other replicas of the family 2^{4-2} there are pairwise interactions that will be modulo equal to each other. Thus, for $k = 4$ and for the same values of k, the number of experiments in the Hartley minimum plan is the same as the number of experiments in the Box minimum plan. Hartley minimum plans require a smaller number of experiments than Box minimum plans to estimate the coefficients of a degree 2 polynomial. However, Hartley plans are inferior to Box plans in the accuracy of estimating these coefficients. In addition, by changing the "star"arm, the Hartley plan cannot be made either rotatable or orthogonal. Hartley plans are reasonable to use when the number of experiments is limited by the experimental conditions; when it is known that some of the effects b_i or b_{ij} are absent in the model (hence, simple effects can be mixed with pairwise interactions without losing the resolving power of the plan); or when it is known apriori that the dispersion of observations is relatively small.

3. Orthogonal CCP of the second order

In general, the second-order CCP is not orthogonal. However, if it is a Box plan, then by changing the star arm and transforming the response function (2), it can be made orthogonal.

Let $\overline{D} = (x_{iu}), i = 1, 2, ..., k, u = 1, 2, ..., N$ be the Box plan matrix, where α and β are constants, and $f(X)$, $f(\widetilde{X})$, $\widetilde{f}(\widetilde{X})$ be the matrix of independent variables corresponding to it and the response function (2). As an example, let us consider the second-order Box CCP for three variables and $n_0 = 1$, whose matrix of independent variables is given in Table 2.As can be seen from Table 1, not all columns of the matrix fulfill the symmetry condition and not all columns are pairwise orthogonal. Indeed, the sums

$$\sum_{u=1}^{N} x_{0u}x_{iu}^2 = \sum_{u=1}^{N} x_{iu}^2 \neq 0, \quad i = 1, 2, \ldots, k;$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 \neq 0, \quad i, j = 1, 2, \ldots, k;\ i \neq j$$

for all rows of the plan.

Table 2: Table 2: Matrix of independent variables

Plan	x_0	x_1	x_2	x_3	x_1x_2	x_1x_3	x_2x_3	x_1^2	x_2^2	x_3^2
FFE 2^3	+	-	-	-	+	+	+	+	+	+
	+	+	-	-	-	-	+	+	+	+
	+	-	+	-	-	+	-	+	+	+
	+	+	+	-	+	-	-	+	+	+
	+	-	-	+	+	-	-	+	+	+
	+	+	-	+	-	+	-	+	+	+
	+	-	+	+	-	-	+	+	+	+
	+	+	+	+	+	+	+	+	+	+
«star»	+	$-\alpha$	0	0	0	0	0	α^2	0	0
	+	α	0	0	0	0	0	α^2	0	0
	+	0	$-\alpha$	0	0	0	0	0	α^2	0
	+	0	α	0	0	0	0	0	α^2	0
	+	0	0	$-\alpha$	0	0	0	0	0	α^2
	+	0	0	α	0	0	0	0	0	α^2
Plan Center	+	0	0	0	0	0	0	0	0	0

To achieve compliance with the symmetry property one should pass from to centered values
$x_i^* = x_i^2 - x_{i,\text{av}}^2$, where $x_{i,\text{av}}^2 = \frac{1}{N}\sum x_{iu}^2$, $i = 1, 2, \ldots, k$.

From Table 2, it is easy to see that the average value $x_{i,\text{av}}^2$ is the same for all x_i^2:

$$x_{i,\text{av}}^2 = c = c(\alpha) = \frac{N_0 + 2\alpha^2}{N}, \quad i = 1, 2, \ldots, k \tag{5}$$

Note that the original (2) and the transformed model are equivalent, since in them all coefficients, except for the zero coefficient, coincide.

After the transformation, the matrix of independent variables for model (2) will be different from the matrix of independent variables X^* for model (5).

It is easy to see that for the transformed model (5) the sums of elements in all columns, except for column x_0, are equal to zero, i.e., the symmetry property is observed in the transformed table. Also, the columns of the matrix X^* , except for the columns of quadratic terms, are orthogonal. That is, only the last k columns of the matrix X^* will be pairwise non-orthogonal for arbitrary values of α :

$$\sum_{u=1}^{N}(x_{iu}^2 - c)(x_{ju}^2 - c) = \sum_{u=1}^{N} x_{iu}^* x_{ju}^* \neq 0, i \neq j \tag{6}$$

The orthogonalization of these columns is achieved by a special selection of the value of α , solving the equation
$\sum_{u=1}^{N} x_{iu}^* x_{ju}^* = N_0(1-c)^2 - 4c(\alpha^2 - c) + (2k-4)c^2 + n_0c^2 = 0; i, j = 1, 2, ..., k, i \neq j.$
Whence

$$N_0 - 2(N_0 + 2\alpha^2)c + c^2(N_0 + 2k + n_0) = N_0 - 2c^2N + c^2N = 0. \tag{7}$$

Hence, $c^2N = N_0$. Then $c = (N_0/N)^{1/2}$.Let's substitute the found value of c into equation (7)
$(N_0/N)^{1/2} = (N_0 + 2\alpha^2)/N$.

From here we find the value of α, which gives the orthogonality property to the Box CCP:

$$\alpha = \sqrt{(\sqrt{N_0N} - N_0)/2} \tag{8}$$

Thus, matrix X^*, will be an orthogonal planning matrix if
$\alpha = \left\{\left[(8 \cdot 15)^{1/2} - 8\right]/2\right\}^{1/2} = 1.215$ and $c = (8/15)^{1/2} = 0.73$.

If x_{iu} is an element of the matrix X^*, the estimates of the regression coefficients are determined by the formula

$$\hat{\beta}_i = \sum_{u=1}^{N} x_{iu}\bar{y}_u \Big/ \sum_{u=1}^{N} x_{iu}^2, \quad i = 1, 2, ..., p. \tag{9}$$

The variance of these estimates

$$D\{\hat{\beta}_i\} = \sigma^2 \Big/ \sum_{u=1}^{N} x_{iu}^2, \quad i = 1, 2, ..., p \tag{10}$$

where σ^2- is the variance of the mean value of the response function at the $u-$th point of the plan.

Estimation of the coefficient

$$\hat{d}_0 = \frac{1}{N}\sum_{u=1}^{N} \bar{y}_u, \tag{11}$$

respectively

$$D\{\hat{d}_0\} = \sigma^2/N. \tag{12}$$

According to (7) $\beta_0 = d_0 - c\sum_{i=1}^{k}\beta_{ii}$. The variances $D\{\hat{\beta}_i$ of the estimates of regression coefficients for second-order plans, unlike linear plans, are different see (10), (12), since they are calculated over different sets of plan points. Estimation of the response function at point $(x_1, x_2, ..., x_k)'$

$$\begin{aligned}\hat{\eta} &= \hat{\beta}_0 + \sum_{1\le i\le k}\hat{\beta}_i x_i + \sum_{1\le i<j\le k}\hat{\beta}_{ij}x_i x_j + \sum_{1\le i\le k}\hat{\beta}_{ii}x_i^2 = \\ &= \hat{d}_0 + \sum_{1\le i\le k}\hat{\beta}_i x_i + \sum_{1\le i<j\le k}\hat{\beta}_{ij}x_i x_j + \sum_{1\le i\le k}\hat{\beta}_{ii}(x_i^2 - c),\end{aligned} \tag{13}$$

and its variance

$$D\{\hat{\eta}\} = \frac{\sigma^2}{N} + \sum_{1\le i\le k} x_i^2 D\{\hat{\beta}_i\} + \sum_{1\le i<j\le k} x_i^2 x_j^2 D\{\hat{\beta}_{ij}\} + \sum_{1\le i\le k}(x_i^2 - c)^2 D\{\hat{\beta}_{ii}\}. \tag{14}$$

Thus, the variance of the response function estimate at some point $(x_1, x_2, \ldots, x_k)'$ depends not only on the distance ρ of this point to the center of the plan, but also on its position on the hypersphere, i.e., the second-order orthogonal plan is not rotatable (Fig. 2).

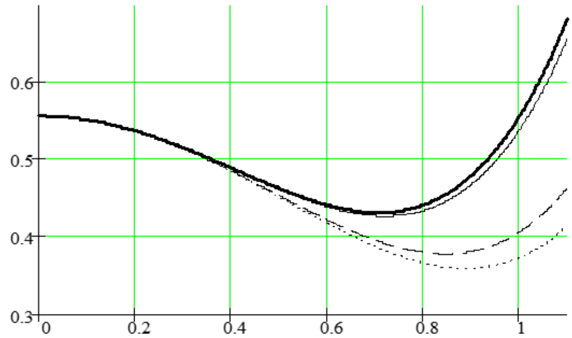

Figure 2: The variance of the response function estimate for the orthogonal Box plan at $k = 2 : 1 - \alpha = 0°, 2 - \alpha = 30°, 3 - \alpha = 45°, 4 - \alpha = 15°$.

Checking the homogeneity of the reproducibility variance, model adequacy, and significance of the polynomial coefficients in the case of using second-order orthogonal CCPs is carried out similarly to the previously discussed scheme.

4. Rotatable second-order CCPs

A plan of order d is called rotatable if the variance of the response function estimate $\eta = (x_1, x_2, \ldots, x_k)$ at a point $(x_1, x_2, \ldots, x_k)'$ depends only on the distance $(x_1, x_2, \ldots, x_k)$ of this point to the center of the plan and does not depend on its position on the hypersphere. Thus, a plan (N) will by definition be rotatable of order d if

$D\{\hat{\eta}(x_1, x_2, ..., x_k)\} = \psi[\rho(x_1, x_2, ..., x_k)]; \quad \rho^2 = \rho^2(x_1, x_2, ..., x_k) = \sum_{i=1}^{k} x_i^2.$

In general, the necessary and sufficient conditions for the existence of rotatable plans of arbitrary order are as follows.

Let $\bar{D} = (x_{iu}) \quad (i = 1, \ldots, k; u = 1, \ldots, N)$ be the plan matrix $\xi(N)$ of order d, and $X = (x_{ju}) \quad (j = 0, 1, \ldots, p; \quad u = 1, \ldots, N)$ be the matrix of independent variables of rank $p + 1$ corresponding to this plan. A plan $\xi(N)$ will be rotatable if and only if the matrix $X'X$ is invariant with respect to the orthogonal transformation R of the plan matrix $\bar{D}$. By invariance of the matrix $X'X$ with respect to the orthogonal transformation R of the plan matrix $\bar{D}$ is meant the condition $X'X = X'^0 X^0$, where X^0 is the matrix of independent variables corresponding to the plan matrix $\bar{D}_0 = \bar{D}R$ and the same response function as the matrix X (the proof is given in [2]). The general form of the matrix X is $X = (E, \bar{D}, B1, B2)$.

An element of the matrix $X'X$ is called a moment. A moment is considered odd if its expression contains at least one odd-degree factor of the form $x_{iu}^{2l+1} (l = 0, 1)$. The necessary and sufficient condition for rotatability of second-order plans is satisfied if all odd moments up to the fourth order are zero and even moments are equal to zero, respectively [2]

$$\sum_{u=1}^{N} x_{iu}^2 = N\lambda_2, \quad i = 1, 2, ..., k; \tag{15}$$

$$\sum_{u=1}^{N} x_{iu}^4 = 3N\lambda_4, \quad i = 1, 2, ..., k; \tag{16}$$

$$\sum_{u=1}^{N} x_{iu}^2 x_{ju}^2 = N\lambda_4, \quad i, j = 1, 2, ..., k; i \neq j. \tag{17}$$

The parameter λ_2 is determined from the condition of plan scale selection, and λ_4 is chosen subject to some constraints.

Thus, it follows that the matrices $\bar{D}$, B_1 and B_2 will be mutually orthogonal, i.e. $\bar{D}'B_1 = \mathbf{0}$, $\bar{D}'B_2 = \mathbf{0}$, $B_1'B_2 = \mathbf{0}$, where $\mathbf{0}$ is the zero matrix. The symmetry condition of the plan $E'\bar{D} = \mathbf{0}$ will also be satisfied.

For the matrix $X'X$ to be nondegenerate, the following condition must be satisfied

$$\frac{\lambda_4}{\lambda_2^2} \neq \frac{k}{k+2}. \tag{18}$$

There is a relation between the number and radii of the hyperspheres on which the points of the rotatable plan lie, on the one hand, and the parameters λ_2 and λ_4, on the other hand. Summarizing by i the equality (15)

$\sum_{u=1}^{N}\sum_{i=1}^{k} x_{iu}^2 = kN\lambda_2$

and using the ratio $\rho_u^2 = \sum_{i=1}^{k} x_{iu}^2$, we obtain

$$\sum_{u=1}^{N} \rho_u^2 = kN\lambda_2, \quad \sum_{\omega=0}^{s} n_\omega \rho_\omega^2 = kN\lambda_2, \tag{19}$$

where $s+1$ is the number of different hyperspheres on which the plan points lie, n_σ is the number of plan points on a hypersphere of radius ρ_ω, with $\sum n_\omega = N$. Summing further on i equality (17) and using (16), we find

$$\sum_{u=1}^{N} x_{ju}^2 \sum_{j=1}^{k} x_{iu}^2 = (k-1)N\lambda_4 + 3N\lambda_4, \quad \sum_{u=1}^{N} \rho_u^2 x_{ju}^2 = (k+2)N\lambda_4. \tag{20}$$

And summarizing by j the equality (20), we obtain

$$\sum_{u=1}^{N} \rho_u^4 = k(k+2)N\lambda_4, \quad \sum_{\omega=0}^{s} n_\omega \rho_\omega^4 = k(k+2)N\lambda_4. \tag{21}$$

Thus, according to (1.19) and (1.21)

$$\frac{\lambda_4}{\lambda_2^2} = \frac{k\sum_{\omega=0}^{s} n_\omega \rho_\omega^4}{(k+2)\left[\sum_{\omega=0}^{s} n_\omega \rho_\omega^2\right]^2}. \tag{22}$$

Then the equality (22) with the last inequality and (18) is transformed into an inequality, and we obtain a constraint on the choice of parameters λ_2 and λ_4: $\frac{\lambda_4}{\lambda_2^2} > \frac{k}{k+2}$.

As can be seen from (22), there are no rotatable plans with points located on only one hypersphere, for in this case $\lambda_4/\lambda_2^2 = k/(k+2)$, i.e., the matrix $X'X$ will be degenerate [see (18)]. Consequently, the points of the rotatable plan must be located on concentric hyperspheres, the number of which is at least two. One of the hyperspheres may be the center point of the plan, i.e., degenerate. In particular, if $s+1 = 2$ and one of the hyperspheres is degenerate, then $\lambda_4/\lambda_2^2 = k(n_1 + n_0)/(k+2)n_1$.

Thus, the following features of the structure of a rotatable plan can be noted:

- the plan must satisfy the symmetry conditions;
- the columns of the plan must be pairwise orthogonal;
- the points of the plan must be located on concentric hyperspheres, the number of which is not less than two.

The general theory of constructing second-order rotatable plans is rather complicated [1, 2]. Since the problem of constructing rotatable plans has no unambiguous solution, we consider only some examples of such plans.

Consider the case when the number of factors $k = 2$. There is a theorem [1] that when $k = 2$, plans for which points are equidistant on a circle of radius $\rho_1 > 0$ and there are n_0

central points will be rotatable if and only if $n_1 > 4$. Thus, by placing points at the vertices of a regular pentagon, hexagon, etc. and adding the required number of center points to them, we obtain a rotatable plan of order 2. Figure 3. shows examples of such plans. The matrices of these plans

$$\bar{D}_1 = \begin{pmatrix} 1 & 0 \\ 0.309 & 0.951 \\ -0.809 & 0.588 \\ -0.809 & -0.588 \\ 0.309 & -0.951 \\ 0 & 0 \end{pmatrix}; \quad \bar{D}_2 = \begin{pmatrix} 1 & 0 \\ 0.5 & 0.866 \\ -0.5 & 0.866 \\ -1 & 0 \\ -0.5 & -0.866 \\ 0.5 & -0.866 \\ 0 & 0 \end{pmatrix}$$

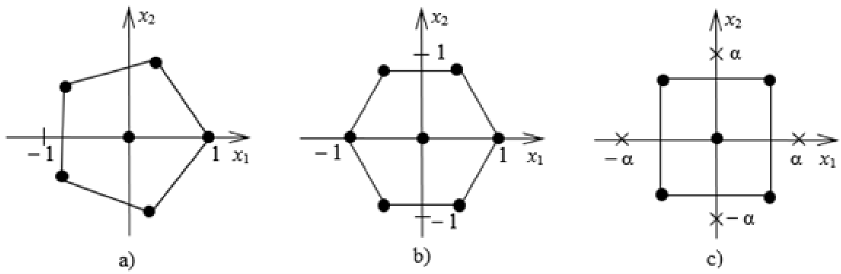

Figure 3: shows an example of another rotatable plan, which is the Box CCP (star shoulder $\alpha = 1.141$)

Let us consider the case $k > 2$. Among the 2nd order rotatable plans, the central composite rotatable plans, which can be obtained from the Box CCP by a special selection of the "star" arm α , are of the greatest practical importance.

Let us give a rule for computing radii of hyperspheres for central composite rotatable plans whose kernel is a FFE of the form 2^k or a FrFE of the form 2^{k-q} (the kernel of the Box plan). The first hypersphere is degenerate. The second hypersphere corresponds to the cube inscribed in it, chosen as the plan kernel. For the kernel $x_i = 1$, hence the radius of this hypersphere is $x_1 = (x_1^2 + x_2^2 + ... + x_k^2)^{1/2} = (k)^{1/2}$.

And the radius of the third hypersphere is the "stellar" arm, which is fitted as follows:$x_2 = \alpha = 2^{(k-q)/4}$.Thus the rotatability of the Box plan is achieved.

Hence, subject to the Box CCP constraints, when $k < 5$, we can use a 2^{k-1} half-replica as the core of the rotatable plan. When $5 \leq k \leq 7$ and $\alpha = 2^{(k-1)/4}$, the rotatable plan will be a minimal Box plan. If $k > 8$, the core of the rotatable plan can be a 1/4-replica ($\alpha = 2^{(k-1)/4}$). In some cases, the radii of the second and third hypersphere coincide , i.e., the number of hyperspheres for such plans is two. Here it is assumed that the number n0 is the same for all the variants. As can be seen, all these plans are unsaturated - the number of estimated parameters is less than the number of experiments.

From the considered examples, we can see that the problem of constructing a rotatable plan does not have a single solution. But in real problems the problem of plan selection usually does not arise, because usually when conducting an experiment there are restrictions both on the total number of experiments (number of plan points) and on their location in space. Also the requirement to the information profile of the plan influences the choice of the plan.

The information about the response surface at a point $(x_1, x_2, \ldots, x_k)'$ is a quantity $1/ND$

where N − is the number of observations at the plan points; D − the variance of the response function estimation at point x. Information is some local measure of the accuracy of the response function estimation attributed to a single observation. The dependence of information on the radius of the hypersphere 111121, on which point x is located, is called the information profile of the plan.

Since λ_2 characterizes the scale of the plan, we can assume without restriction of generality that $\lambda_2 = 1$. For this case, it is shown in [2] that for (13), using the inverse matrix , we can obtain,

$$ND\{\hat{\eta}_x\} = A\sigma^2\{2(k+2)\lambda_4 + 2\lambda_4(\lambda_4 - 1)(k+2)\rho^2 + [(k+1)\lambda_4 - (k-1)]\rho^4\} \tag{23}$$

where $A = 1/\{2\lambda_4[(k+2)\lambda_4 - k]\}$.

Expression (23) can be written in the form of dependence

$$\frac{1}{ND\{\hat{\eta}_x\}} = \psi(\sigma^2; k; \lambda_4; \rho),$$

representing the information profile of the rotatable plan of the 2nd order. k, σ^2, λ_4 are the parameters defining the profile of the plan. For a given k and for different λ_4, different information profiles can be obtained. Since $\lambda_2 = 1$, the parameter λ_4 is related to the total number of observations N by the relation (22).

Often one is interested in information about the response function in some neighborhood of the plan center. In this case, the profile of the plan is chosen such that the information is nearly constant inside a hypersphere of radius $\rho = 1$. Such planning is called uniform-rotatable planning. To obtain such planning, it is sufficient to ensure equality of the variance at the center of the plan ($\rho = 0$) and on the surface of the hypersphere of radius $\rho = 1$. According to (23), the parameter λ_4 should be taken equal to the positive root of the following quadratic equation:

$$2\lambda_4(\lambda_4 - 1)(k+2) + \lambda_4(k+1) - (k-1) = 0 \tag{24}$$

There always exists λ_4 found from (24) such that $\lambda_4 > k/(k+2)$. But at the same time, the parameter λ_4 must satisfy the condition (22) and usually it is not possible to satisfy both conditions at once, so to obtain uniform-rotatable planning, by selecting the number of observations $n0$ in the center of the plan, one achieves that the parameter λ_4, determined by the equality (22), is close to the value found from (24).

5. Discussion of results

Consider the rotatable plan ($k = 2$) shown in Fig. 3, b). From (22) we have $\lambda_4 = (n_1 + n_0)/2n_1$.

Suppose that $n_0 = 6$. Since $n_1 = 6$, then $N = 12$, and $\lambda_4 = 1$. Using (23) and $\mu\sigma^2 = 1$, we have

$$\frac{1}{ND\{\hat{\eta}_x\}} = \frac{1}{2 + \rho^4/2}$$

And from (24) we obtain $\lambda_4 = 0,784$ for uniform-rotatable planning. When the number of observations in the center of the plan n_0 changes, the information profile of the plan changes. By selecting n0, we achieve uniform-rotatable planning. Fig. 4 shows the corresponding information profiles of the plans.

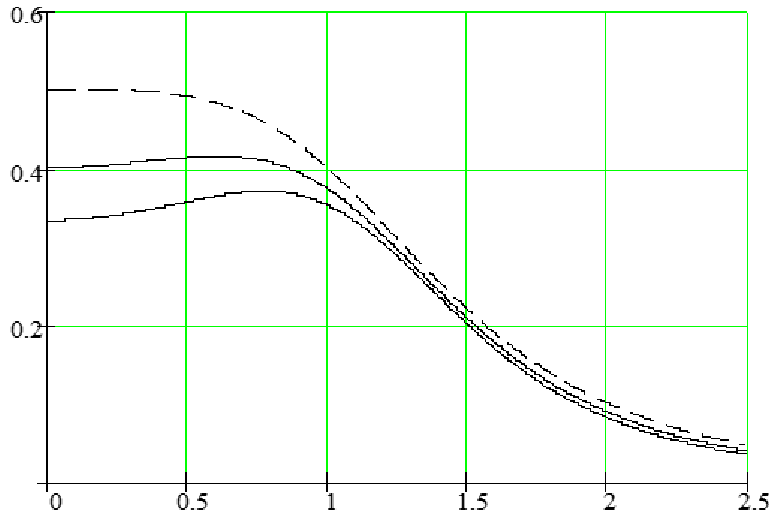

Figure 4: Information profiles of plans:$1-\delta_4 = 1 (n_0 = 6)$; uniform-rotatable planning: $2-\delta_4 = 0.83 (n_0 = 4)$; $3-\delta_4 = 0.75 (n_0 = 3)$

For the parameters of the model (2) and their variance (covariance) under rotatable scheduling, the following expressions are obtained [2]:

$$\hat{\beta}_0 = \frac{A}{N}\left[2\lambda_2^2(k+2)\sum_{n=1}^{N} y_n - 2\lambda_2\lambda_4 \sum_{i=1}^{k}\sum_{n=1}^{N} x_{in}^2 y_n\right]$$

$$\hat{\beta}_i = \frac{1}{\lambda_2 N}\sum_{n=1}^{N} x_{in}y_n; \quad \hat{\beta}_{ij} = \frac{1}{\lambda_2 N}\sum_{n=1}^{N} x_{in}x_{jn}y_n$$

$$\hat{\beta}_{ii} = \frac{A}{N}\left[(k+2)\lambda_2 - k\lambda_2^2 \sum_{n=1}^{N} x_{in}^2 y_n + (\lambda_2^2 - \lambda_4)\sum_{i=1}^{k}\sum_{n=1}^{N} x_{in}^2 y_n - 2\lambda_2\lambda_4 \sum_{n=1}^{N} y_n\right]$$

$$D\{\hat{\beta}_0\} = \frac{\sigma^2}{N}2\lambda_2^2(k+2)A; \quad D\{\hat{\beta}_i\} = \frac{\sigma^2}{\lambda_2 N}; \quad D\{\hat{\beta}_{ij}\} = \frac{\sigma^2}{\lambda_2 N}$$

$$D\{\hat{\beta}_{ii}\} = \frac{\sigma^2}{N}\left[(k+1)A_4 - (k-1)\lambda_2^2\right]A; \quad \lambda_2 = \frac{1}{N}\sum_{n=1}^{N} x_{in}^2; \quad \lambda_4 = \frac{1}{3N}\sum_{n=1}^{N} x_{in}^4$$

$$\text{cov}\{\hat{\beta}_0, \hat{\beta}_{ii}\} = -\frac{\sigma^2}{N}2\lambda_4 A; \quad \text{cov}\{\hat{\beta}_{ii}, \hat{\beta}_{jj}\} = \frac{\sigma^2}{N}(1-\lambda_4)A.$$

The remaining covariances are equal to zero. These formulas are valid for 2nd order rotatable planning for any number of independent variables.

When λ_4, the rotatable planning turns out to be almost orthogonal, only the covariance is not zero $\text{cov}\{\hat{\beta}_0, \hat{\beta}_{ii}\}$. But the value of λ_4 depends on the type of information profile of the plan, which requires that $\lambda 4$ be slightly less than unity in order to obtain uniform-rotatable planning. And this leads to a further loss of orthogonality - become different from zero and $\text{cov}\{\hat{\beta}_{ii}, \hat{\beta}_{jj}\}$. Checking the homogeneity of the reproducibility variance, model adequacy and significance of the model coefficients is done according to the scheme discussed earlier [12-14].

Let repeated observations $\{y_{0u}\}$, $u = 1, 2, \ldots, n_0$, exist only in the center of the plan. Let us denote by $y_1, y_2, \ldots, y_N$ the observations at the points of the plan. Then $y_{0u} = y_{(N-n_0)+u}$, $u = 1, 2, \ldots, n_0$. The value

$$Q_2 = \sum_{u=1}^{n_0} (y_{0u} - \bar{y}_0)^2,$$

where $\bar{y}_0 = \frac{1}{n_0} \sum_{u=1}^{n_0} y_{0u}$, is due to the variance of the observation errors, so the value of

$$s_e^2 = Q_2/(n_0 - 1)$$

will be an unbiased estimate of the variance of the observation errors σ^2. The sum of squares due to model inadequacy is $Q_1 = Q_0 - Q_2$, where the residual sum of squares $Q_0 = Y^T Y - \hat{\beta}^T Y$, and $\hat{\beta} = (X^T X)^{-1} X^T Y$. When the hypothesis of model adequacy is true, the value of

$$s_r^2 = Q_1/[n - (p + 1)],$$

where $n = N - n_0 + 1$ is the number of different points of the plan; $p + 1 = (k+1)(k+2)/2$ is the number of estimated parameters, will be the unbiased estimate of the parameter σ^2. And the hypothesis of model adequacy is rejected if

$$s_r^2/s_e^2 > F_\alpha(n - (p + 1), n_0 - 1),$$

where $F_\alpha(n - (p + 1), n_0 - 1)$ is the quantile of the level α of the Fisher distribution with the number of degrees of freedom $n - (p + 1)$ and $n_0 - 1$.

6. Conclusions

In the work the methods of the theory of experiment planning are considered and studied in detail. The methods of statistical data processing are given. At the same time, the formulation of the problem of processing data obtained empirically is formulated. The solution of the problem is given by the method of least squares. The analysis of the obtained regression model is also presented. The procedure of testing the hypothesis of model adequacy is given. The criteria of optimal planning are formulated. The formulation of the optimization problem is given. The construction of full factor experiments of 2^k type is also studied. The procedure of processing the results of experiments is presented. The peculiarities of construction of fractional factor experiment are considered. Linear plans, differences in their purpose and application from full factor experiments and fractional factor experiments are also presented. D -optimal plans are presented in detail, among them exact and continuous D - optimal plans; continuous D - optimal plans for quadratic regression on the hypercube; exact plans close to -optimal plans. Substantial attention is given to the issues of second-order central composite plans for building quadratic models. The structure of central composite plans is given. Box, Hartley plans are studied. Methods of obtaining orthogonal and rotatable second-order central composite plans from Box plans are considered. The theorem on rotatability of the second-order central composite plan is formulated.

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