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SEQUENTIAL DESIGN OF EXPERIMENTS CONSISTING OF MEASUREMENTS IN SEVERAL EXPERIMENTAL POINTS

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In their paper[1] Box and Hunter proved a furmula (formula (7) in this paper) which has been used for the design of experiments[1,2] in the case of measuring in only one experimental point. The puprose of this is to investigate a more general case when:

a) An estimate $\hat{\vec{\theta}}$ of $\vec{\theta}$ and the corresponding dispersion matrix D are known before the planning;

b) The planned experiment consists of stochastically independent measurements taken in several experimental points.

A design which is based on the results of some previous experiments (assumption a)) differs from designs proposed for instance in[3-5].

The case of correlated experimental data is mentioned in theorem 2.

It is reasonable to call the proposed design a sequential design of experiments, because in the scheme:

... - experiment- analysis- design- experiment- ...

the results of the previous experiments influence the design of a new experiment by means of the dispersion matrix D .

The usefulness of a sequential can be demonstrated by the NN - scattering experiments, where the purpose of many expensive experiments is only to obtain more precise results than the old one.

The problem of the optimal distribution of the measuring time (or the price of the experiment) between the measurements in different experimental points will be investigated in detail. It will be proved, that the solution of such a problem is unique (theoren 3). A solution in an analytical form will be given in the case of long measurement times.

Some generalization of the continuous planning of experiments[8] will be given.

The investigated design of experiments fits the following structure: n is a fixed integer, $f(x_1),\ldots,f(x_n)$ are linearly inderpendent $m\times 1$ vectors $(m\geq n)$. Let t_i denote the time of the measurement in the experimental point x_i $(i=\overline{1,n})$. The result of the measurement in the point x_i is y_i; let us assume: $E(y_i)=\vec{f}(x_i)\vec{\theta}$ $D(y_i)=1/\lambda_i t_i$. Here λ_i is a known positive constant - the efficiency of the measurement in x_i and the prime denotes the transposition of a vector. The experimenter does not know the value of the vector $\vec{\theta}=\|\theta_1,\ldots,\theta_m\|$ but he knows an unbiassed estimate $\hat{\vec{\theta}}$ and the corresponding $m\times m$ nonsingular dispersion matrix $D(D_{ij} = E\{(\hat{\theta}_i-\theta_i)(\hat{\theta}_j-\theta_j)\})$.

A desidn of an experiment specifies the experimental points $x_1,\ldots,x_n$ (that is $\vec{f}(x_i)$ and λ_i) and the measurement times $t_1,\ldots,t_n$. The used criterion for optimality is the variance of the best liner estimate of some variable:

$$y_0=\vec{f}'(x_0)\vec{\theta}. \tag{1}$$

The optimal design must satisfy the conditions $\sum_{i=1}^{n}p_i^2t_i=T$ and $0\leq\alpha_i\leq t_i\leq\beta_i$ $(i=\overline{1,n})$ where α_i and β_i are given numbers, T is the price of the whole experiments and p_i^2 is the price of the i-th measurement in a time unit.

N o t e If $E(y_i)=\eta_i(\vec{\theta})$ is a nonlinear function, we must use the following approximation:

$$E(y_i)=\vec{f}(x_i)\,\vec{\theta}+r_i \tag{2}$$

where

$$f_j(x_i)=\frac{\partial\eta_i(\vec{\theta})}{\partial\theta_j}\Big|_{\vec{\theta}=\hat{\vec{\theta}}},\qquad r_i=\eta_i(\hat{\vec{\theta}}). \tag{3}$$

The following notation will be used throughout the paper: $D(\vec{t})$ is the $m\times m$ dispersion matrix of the best linear estimate of $\vec{\theta}$ (i.e. the error matrix, or the matrix inverse to the information matrix /8/), where $\vec{t}'=\|t_1,\ldots,t_n\|$. $V(\vec{t})$ is the $(n+1)\times(n+1)$ covariance matrix of the best linear estimates of $y_0,y_1,\ldots,y_n$:

$$V_{ij}(\vec{t})=\vec{f}'(x_i)D(\vec{t})\vec{f}(x_j)\quad i,j=\overline{0,n} \tag{4}$$

σ is the $(n+1)\times(n+1)$ covariance matrix of $y_0,\ldots,y_n$:

$$\sigma_{ij}=0 \quad \text{if } i=0 \text{ or } j=0$$
$$=\frac{1}{\lambda_i t_i}\delta_{ij} \quad \text{if } i,j=1,\ldots,n \tag{5}$$

$$(\delta_{ij}=1 \text{ if } i=j;\ \delta_{ij}=0 \text{ if } i\neq j).$$

We shall use the abbreviations:

$$D(\vec{0}) = D, \quad V(\vec{0}) = V \tag{6a}$$

for the values before the experiment, and

$$D(t_1,0,\dots,0) = D(t_1), \quad V(t_1,0,\dots,0) = V(t_1) \tag{6b}$$

for the values after the first meaurement.

The following result is due to Box and Hunter [1]:

T h e o r e m 1. If the measurement is taken in only one experiment point then:

$$D(t_1) = D\,\frac{1+\lambda_1 t_1[\vec{f}'(x_1)D\vec{f}(x_1) - \vec{f}(x_1)\vec{f}'(x_1)D]}{1+\lambda_1 t_1 \vec{f}'(x_1)D\vec{f}(x_1)} . \tag{7}$$

Corollary. From (4), (5) and (7) we get:

$$V_{ij}(t_1) = \frac{V_{ij}(V_{11}+\sigma_{11}) - (V_{i1}+\sigma_{i1})(V_{1j}+\sigma_{1j})}{V_{11}+\sigma_{11}} \tag{8}$$

L e m m a 1.

Let us denote $k_i\ (0<k_i<n,\ i=\overline{1,r})$ r different integers one of which is equal to 1. Then:

$$|V_{ij}+\sigma_{ij}|_{i,j=k_1,\dots,k_r} = (V_{11}+\sigma_{11})\,|V_{ij}(t_1)+\sigma_{ij}|_{\substack{i,j=k_1,\dots,k_r\\ i,j\neq 1}} . \tag{9}$$

P r o o f. Let us denote: $A_{ij} = V_{ij}+\sigma_{ij}$. We obtain from (8)

$$|V_{ij}(t_1)+\sigma_{ij}|_{\substack{i,j=k_1,\dots,k_r\\ i,j\neq 1}} = \frac{1}{A_{11}^{k-1}}\,|A_{11}A_{ij} - A_{i1}A_{1j}|_{\substack{i,j=k_1,\dots,k_r\\ i,j\neq 1}} . \tag{10}$$

The determinant on the right side of (10) is equal to a sum of determinants, the first of which is equal to $|A_{11}A_{ij}|_{i,j=k_1,\dots,k_r,\ i,j\neq 1}$ and the others are obtained by substituting the column-vector $\|-A_{i1}A_{1\ell}\|_{\substack{i=k_1,\dots,k_r\\ i\neq 1}}$ for the ℓ-th column of the first determinant. We obtain:

$$|V_{ij}(t_1)+\sigma_{ij}|_{\substack{i,j=k_1,\dots,k_r\\ i,j\neq 1}} = \frac{1}{A_{11}^{k-1}}\{|A_{11}A_{ij}|_{\substack{i,j=k_1,\dots,k_r\\ i,j\neq 1}}$$

$$- \sum_{\substack{\ell = k_1, \dots, k_r \\ \ell \neq 1}} |A_{11} A_{ik_1}, \dots, A_{11} A_{ik_{\ell-1}}, A_{11} A_{i\ell}, A_{11} A_{ik_{\ell+1}}, \dots, A_{11} A_{ik_r}|_{\substack{i = k_1, \dots, k_r \\ i \neq 1}} \} =$$

$$= \frac{1}{A_{11}} \sum_{\ell = k_1, \dots, k_r} (-1)^{\ell - 1} A_{1\ell} |A_{ij}|_{\substack{i,j = k_1, \dots, k_r \\ i \neq 1, j \neq \ell}} = \frac{1}{A_{11}} |A_{ij}|_{i,j = k_1, \dots, k_r} . \tag{11}$$

Q.E.D.

T h e o r e m 2. Let the variables $y_1, \dots, y_n$ be correlated and let be $\sigma_{ij} = E\{[y_i - \vec{f}'(x_i)\vec{\theta}][y_j - \vec{f}'(x_j)\vec{\theta}]\}$ $(i,j = \overline{1,n})$. Then the variance of the estimate of $y_0 = \vec{f}'(x_0)\vec{\theta}$ can be written as:

$$V_{00}(\vec{t}) = \frac{|V_{ij} + \sigma_{ij}|_{i,j=0}^{n}}{|V_{ij} + \sigma_{ij}|_{i,j=1}^{n}} \tag{12}$$

P r o o f. The assumption that D is definite positive is sufficient for the fraction in (12) to exist.

Consider first the case of uncorelated $y_1, \dots, y_n$. For $n = 1$ formula (12) is identical with (8). If (12) is correct for $n = k$ it is also correct for $n = k+1$. We can demonstrate this, it we include the first measurement (with the measurement time t_1) to the "old" experiments. We obtain:

$$V_{00}(t_2, \dots, t_{k+1}) = \frac{|V_{ij}(t_1) + \sigma_{ij}|_{i,j=0,\ i,j \neq 1}^{k+1}}{|V_{ij}(t_1) + \sigma_{ij}|_{i,j=2}^{k+1}}$$

and from this and (9) follows (12).

We can go over to the case of correlated measurements using an orthogonal transformation. We shall use for this the following notations:

1. $\sigma^{(0)} = \| \sigma_{ij} \|$

2. $C^{(0)}$ is an orthogonal matrix which satisfies the following equality:

$$C^{(0)'} \sigma^{(0)} C^{(0)} = H^{(0)} \tag{13}$$

where $H^{(0)}$ is a diagonal matrix.

3. C is a $(n+1)\times(n+1)$ matrix:

$C_{00}=1,\quad C_{0i}=C_{i0}=0\quad \text{for}\quad i=\overline{1,n}$

$C_{ij}=C^{(0)}_{ij}\quad \text{for}\quad i,j=\overline{1,n}.$

4. F is the following $m\times(n+1)$ matrix:

$$F_{ij}=f_i(x_j)\quad i=\overline{1,m},\ j=\overline{0,n}$$

and

$$F^{(0)}=\|F_{ij}\|^{n}_{i,j=1}$$

5. We obtain the vectors $\vec{g}(x_0),\dots,\vec{g}(x_n)$ from $\vec{f}(x_0),\dots,\vec{f}(x_n)$ by means of the transformation

$$G=F\,C \tag{14}$$

where

$$G=\|\vec{g}(x_0),\dots,\vec{g}(x_n)\|.$$

It follows from (14) and the linear independence of $\vec{f}(x_1),\dots,\vec{f}(x_n)$ that $\vec{g}(x_1),\dots,\vec{g}(x_n)$ are linearly independent too, and that $\vec{g}(x_0)=\vec{f}(x_0)$.

The described transformation does not influence the dispersion matrix $D(\vec{t})$. This can be demostrated by substituting (13) and (14) into a known equation (the sum of the information matrices/8/):

$$D^{-1}(t)=D^{-1}+F^{(0)\prime}\sigma^{(0)}F^{(0)}. \tag{15}$$

Using (15), the equality $\vec{g}(x_0)=\vec{f}(x_0)$ and the correctness of (12) for the uncorrelated case, we obtain:

$$V_{00}(\vec{t})=\vec{f}'(x_0)D(\vec{t})\vec{f}(x_0)=$$

$$=\vec{g}'(x_0)D(\vec{t})\vec{g}(x_0)=\frac{|V^{g}+H|}{|V^{(0)g}+H^{(0)}|} \tag{16}$$

where $V^{g}=G'HG,\quad V^{(0)g}=\|V^{g}_{ij}\|^{n}_{i,j=1}$

and

$H_{0i}=H_{i0}=0\quad \text{for}\quad i=\overline{0,n}$

$H_{ij}=H^{(0)}_{ij}\quad \text{for}\quad i,j=\overline{1,n}$

Using the orthogonality of C we obtain

$$|V^{g}+H|=|G'DG+H|=|C'[F'DF+CHC']C|=|V^{f}+\sigma| \tag{17}$$

and

$$|V^{(0)9}+H^{(0)}|=|V^{(0)f}+\sigma^{(0)}|. \tag{18}$$

Substituting (17) and (18) into (16) we obtain the statement of the theorem.

<u>Corollary 1.</u> In an analogical way as in the theorem 2, we can demonstrate the following statement: If $y_0=\vec{f}'(x_0)\vec{\theta}$ and $u_0=\vec{\phi}'(x_0)\vec{\theta}$

then

$$\mathrm{cov}[y_0,u_0;\vec{t}]=\vec{f}'(x_0)D(\vec{t})\vec{\phi}(x_0)=\frac{|V_{ij}+\sigma_{ij}|^{n}_{i,j=0}}{|V_{ij}+\sigma_{ij}|^{n}_{i,j=1}}$$

where we must substitute $\vec{f}'(x_i)D\vec{\phi}(x_0)$ for $V_{i0}(i=\overline{0,n})$ in (4).

<u>Corollary 2.</u> It is useful to write the time dependence of $V_{00}(\vec{t})$ in an explicit form in the case of uncorrelated $y_1,\dots,y_n$. Taking into acount, that $\sigma_{ij}=\delta_{ij}/\lambda_i t_i \quad (i=\overline{1,n})$ we can expand the numerator and demominator of (12) in terms $\prod_i \lambda_i t_i$. We obtain:

$$V_{00}(\vec{t})=\frac{V_{00}+\sum_{r=1}^{n}\sum_{\substack{k_1,\dots,k_r=1\\ k_1<\dots<k_r}}^{n}|V_{ij}|_{i,j=0,k_1,\dots,k_r}\lambda_{k_1}t_{k_1}\dots\lambda_{k_r}t_{k_r}}{1+\sum_{r=1}^{n}\sum_{\substack{k_1,\dots,k_r=1\\ k_1<\dots<k_r}}^{n}|V_{ij}|_{i,j=k_1,\dots,k_r}\lambda_{k_1}t_{k_1}\dots\lambda_{k_r}t_{k_r}}. \tag{19}$$

It will be supposed in the sequal, that the experimental data $y_1,\dots,y_n$ are uncorrelated.

The general design problem (including the choise of the optimum points x_i) is difficult, since the way of solving it will depend on the form of $\vec{f}(x_i)$ as a function of x_i. For this reason we investigate in a general way only the method of fitting $t_1,\dots,t_n$ assuming, that the x_i are fixed (i.e. $\vec{f}(x_i)$) and λ_i are fixed). The problem of the optimal fitting of x_i is mentioned at the end of the paper.

<u>Theorem 3.</u> Let D be definite positive, $\vec{f}(x_1),\dots,\vec{f}(x_n)$ linearly independent, $y_1,\dots,y_n$ uncorrelated. Let $\alpha_i, \beta_i \; (i=\overline{1,n})$ be given positive numbers.

Then:

1. $$\frac{\partial V_{00}(\vec{t})}{\partial t_s}=-\lambda_s V_{0s}^2(\vec{t}) \tag{21}$$

and α_i, β_i

$$\frac{\partial^2 V_{00}(\vec{t})}{\partial t_r \partial t_s} = 2\lambda_r V_{0r}(\vec{t}) V_{rs}(\vec{t}) V_{s0}(\vec{t}) \lambda_s \tag{22}$$

2. The matrix of the second derivatives

$$M = \left\| \frac{\partial^2 V_{00}(\vec{t})}{\partial t_r \partial t_s} \right\|^n_{r,s=1} \tag{23}$$

is semidefinitive positive for all $\vec{t}$ and is definite positive in the point where $V_{00}(\vec{t})$ is extremal under the condition $\Sigma^n_{i=1} p^2_i t_i = T$.

3. Excluding the trivial case: $V_{0i}(\vec{t}) = 0$ for all i: $1 \leq i \leq n$ (the measurements give no information) a unique extremum (minimum) of the function $V_{00}(\vec{t})$ under the condition $\Sigma^n_{i=1} p^2_i t_i = T$ exists.

4. In the nontrivial case a unique minimum of $V_{00}(\vec{t})$ under the conditions: $\Sigma^n_{i=1} p^2_i t_i = T$, $\beta_k \geq t_k \geq \alpha_k$ $(k = \overline{1, n})$ exists.

P r o o f.

1. From

$$D^{-1}(\vec{t})\, D(t) = I$$

where I is a unit matrix, we obtain:

$$\frac{\partial D^{-1}(\vec{t})}{\partial t_s} D(\vec{t}) + D^{-1}(\vec{t}) \frac{\partial D(\vec{t})}{\partial t_s} = 0. \tag{24}$$

The derivatives $\frac{\partial D^{-1}(\vec{t})}{\partial t_s}$ can be obtained from (15), which for uncorrelated measurements takes the form:

$$D^{-1}(t) = D^{-1} + \sum_{i=1}^{n} \vec{f}(x_i) \vec{f}'(x_i) \lambda_i t_i$$

Substituting these derivatives into (24) we obtain:

$$\frac{\partial D(\vec{t})}{\partial t_s} = -\lambda_s D(\vec{t}) \vec{f}(x_s) \vec{f}'(x_s) D(\vec{t}).$$

Multiplying this by $\vec{f}'(x_0)$ and $\vec{f}(x_r)$ we obtain:

$$\frac{\partial V_{0r}(\vec{t})}{\partial t_s} = -\lambda_s V_{0s}(\vec{t}) V_{sr}(\vec{t}) \tag{25}$$

Derivating (25) once more we get (22).

2. We shall use the Lagrange method to calculate the extremal points of $V_{00}(\vec{t})$ subject to the condition $\Sigma_{i=1}^{n} p_i^2 t_i = T$. Applying (22) we get the following equations (with respect to $\vec{t}$ and μ):

$$-\lambda_i V_{0i}^2(\vec{t}) + \mu p_i^2 = 0 \qquad i = \overline{1,n}$$

$$\sum_{k=1}^{n} p_k^2 t_k = T$$

Eliminating the constant μ from these equations, we obtain:

$$V_{0i}^2(\vec{t}) = \frac{p_i^2}{\lambda_i T} \sum_{k=1}^{n} \lambda_k V_{0k}^2(\vec{t}) t_k \qquad i = \overline{1,n} \tag{26}$$

Since D is definite positive and $\vec{f}'(x_1), \ldots, \vec{f}(x_n)$ are linearly independent, it follows from (4), that $\| V_{rs}(t) \|_{r,s=1}^{n}$ is definite positive. It follows from this and (22), that M is semidefinite positive. It follows from (26) that in the extremal point $V_{0i}(\vec{t}) \neq 0$ for $i = \overline{1,n}$ in the nontrivial case, so that the quadratical form:

$$\sum_{r,s=1}^{n} c_r M_{rs} c_s$$

can be equal to zero only if $c_r = 0$ for all r.

3. If follows from the positive definiteness (semidefiniteness) of M that the second derivative of $V_{00}(\vec{t})$ taken in an arbitrary direction in the space of the vectors $\vec{t}$ is positive (nonnegative). For this reason $V_{00}(\vec{t})$ has a unique extremum under the condition $\Sigma_{i=1}^{n} p_i^2 t_i = T$ which is a minimum.

4. Let us denote the solution of (26) $\tau_1, \ldots, \tau_n$ und let

$$\tau_i < \alpha_i \qquad \text{for} \qquad i = \overline{1,s}$$

$$\tau_j > \beta_j \qquad \text{for} \qquad j = \overline{s+1, r}$$

$$\alpha_k \le \tau_k \le \beta_k \quad \text{for} \quad k = \overline{r+1, n} \; .$$

Let $\vec{\mu}$ be an arbitrary point of the space of the vectors $\vec{t}$ such that $\mu_1 > \alpha_1$. Let us denote by $\vec{v}$ the point in which the line going through $\vec{\mu}$ and $\vec{\tau}$ intersects the hyperplane $t_1 = \alpha_1$. From the part 2 of the theorem 3 we get:

$$V_{00}(\vec{v}) \le V_{00}(\vec{\mu})$$

i.e. the extremal point of $V_{00}(\vec{t})$ is in the hyperplane $t_1 = \alpha_1$. Since the same concideration is valid for $t_2, \ldots, t_r$ the optimal point lies in the intersection of r hyperplanes: $t_i = \alpha_i$ $(i = \overline{1, s})$ and $t_j = \beta_j$ $(j = \overline{s+1, r})$.

After substituting $\alpha_1, \ldots, \alpha_s, \beta_{s+1}, \ldots, \beta_r$ for $t_1, \ldots, t_r$ into (19), we repeat the considerations of part 3 of the proof for $n - r$ experimental points, i.e. we minimize $V_{00}(\alpha_1, \ldots, \alpha_s, \beta_{s+1}, \ldots, \beta_r, t_{r+1}, \ldots, t_n)$ with respect to $t_{r+1}, \ldots, t_n$ and subject to the condition

$$\sum_{i=r+1}^{n} p_i^2 t_i = T - \sum_{i=1}^{s} \alpha_i p_i^2 - \sum_{i=s+1}^{r} \beta_i p_i^2$$

and so on. After a finite amount of such interactions we obtain:

a) either all t_i are equal to α_i (β_i),

b) or some t_i are obtained by the Lagrange method, which gives a unique solution.

The theorem is proved.

<u>The solution for large measurement times.</u>

<u>Lemma 2.</u> If U is a definite positive $p \times p$ matrix and

$$U^{(k)} = \| U_{ij} \|_{\substack{i,j=1 \\ i,j \neq k}}^{p} \qquad (1 \leq k \leq p) \tag{27}$$

then

$$U_{ij}^{(k)-1} = U_{ij}^{-1} - \frac{U_{ik}^{-1} U_{kj}^{-1}}{U_{kk}^{-1}} \tag{28}$$

<u>Proof.</u> For $s \neq k$ we can write:

$$\sum_{\substack{j=1 \\ j \neq k}}^{p} \left(U_{ij}^{-1} - \frac{U_{ik}^{-1} U_{kj}^{-1}}{U_{kk}^{-1}} \right) U_{js} = \sum_{\substack{j=1 \\ j \neq k}}^{p} U_{ij}^{-1} U_{js} - \frac{U_{ik}^{-1}}{U_{kk}^{-1}} \left(\sum_{j=1}^{p} U_{kj}^{-1} U_{js} - U_{kk}^{-1} U_{ks} \right) =$$

$$= \sum_{j=1}^{p} U_{ij}^{-1} U_{js} = \delta_{is}$$

<u>Corollary.</u> If $X = \| U_{ij} \|_{i,j=1}^{r}$ $(r \leq p)$ such numbers α, β exist, that $0 \leq \alpha \leq \beta \leq 1$ and that:

$$\frac{|X|_{\substack{i,j=1 \\ i,j \neq s}}^{r}}{|X|_{i,j=1}^{r}} = X_{ss}^{-1} = \alpha U_{ss}^{-1} \qquad (s \leq r) \tag{29a}$$

and

$$\frac{|X|_{\substack{i,j=1 \\ i,j \neq s,g}}^{r}}{|X|_{\substack{i,j=1 \\ i,j \neq g}}^{r}} = X_{ss}^{(g)-1} = \beta U_{ss}^{-1} \qquad (s, g \leq r,\ s \neq g) \tag{29b}$$

L e m m a 3. If $\| V_{ij} \|_{i,j=0}^{n}$ is non-singular and

$$t = \frac{a}{n} \frac{V_{rr}^{-1}}{\lambda_r} \qquad (r=\overline{1,n}) \tag{30}$$

where a is a given number: $a > 1$, then such numbers b_r and c_r exist that : $a \leq b_r \leq c_r$ and that the following equalities are valid:

$$\sum_{\substack{k_1,\dots,k_{r-1}=1 \\ k_1<\dots<k_{r-1}}}^{n} | V_{ij} |_{i,j=0,k_1,\dots,k_{r-1}} \prod_{i=k_1,\dots,k_{r-1}} \lambda_i t_i =$$

$$= \frac{1}{b_r} \sum_{\substack{k_1,\dots,k_r=1 \\ k_1<\dots<k_r}}^{n} | V_{ij} |_{i,j=0,k_1,\dots,k_r} \prod_{i=k_1,\dots,k_r} \lambda_i t_i \tag{31}$$

and

$$\sum_{\substack{k_1,\dots,k_{r-1}=1 \\ k_1<\dots<k_{r-1}}}^{n} | V_{ij} |_{i,j=k_1,\dots,k_{r-1}} \prod_{i=k_1,\dots,k_{r-1}} \lambda_i t_i =$$

$$= \frac{1}{c_r} \sum_{\substack{k_1,\dots,k_r=1 \\ k_1<\dots<k_r}} | V_{ij} |_{i,j=k_1,\dots,k_r} \prod_{i=k_1,\dots,k_r} \lambda_i t_i \tag{32}$$

P r o o f. Substituting V for U in the lemma 2 we obtain from (30) and (29a):

$$| V_{ij} |_{i,j=0}^{r} \lambda_r t_r \frac{a}{a} = \frac{1}{n} | V_{ij} |_{i,j=0}^{r-1} . \tag{33}$$

Let us define: $b_r = \frac{a}{a}$. Multiplying (33) by $\prod_{i=1}^{r-1} \lambda_i t_i$, substituting k_i for i (for $i=\overline{1,r}$) and taking the sum $\sum_{k_1,\dots,k_r=1}^{n}$ we obtain (31).

Formula (32) can be obtained from (29b) analogously.

T h e o r e m 4. If

1. $| V_{ij} |_{i,j=0}^{n} \neq 0$

2. $$T \geq \frac{a}{n} \left(\max_{1\leq s\leq n} \frac{p_s V_{ss}^{-1}}{\sqrt{\lambda_s} | V_{s0}^{-1} |} \right) \sum_{i=1}^{n} \frac{| V_{k0}^{-1} |}{\sqrt{\lambda_k}} p_k \tag{34}$$

where a is a given number: a > 1.

Then:

1. In the n -dimensional region:

$$\Omega_a = \{ \vec{t} : t_s \geq \frac{a}{n} \frac{V^{-1}_{ss}}{\lambda_s}; \ (s = \overline{1,n}) \}$$

the function $V_{00}(\vec{t})$ can be oproximated by the function:

$$W_{00}(\vec{t}) = \frac{1}{V^{-1}_{00}} \cdot e^{\sum_{k=1}^{n} \frac{1}{\lambda_n t_m} \frac{(V^{-1}_{0k})^2}{V^{-1}_{00}}} \tag{35}$$

The accuracy i of this approximation is estimated by the relation

$$\frac{|W_{00}(\vec{t}) - V_{00}(\vec{t})|}{V_{00}(\vec{t})} < \frac{1}{a^2 - 1} \tag{36}$$

2. The fuction $W_{00}(\vec{t})$ attains'its minimum in Ω_a subject to the condition $\Sigma_{i=1}^{n} p_i^2 t_i = T$ at the point $\vec{r}' = || r_1, \ldots, r_n ||$ where:

$$r_s = T \frac{|V^{-1}_{0s}|}{\sqrt{\lambda_s}\, p_s} \Big/ \sum_{k=1}^{n} \frac{p_k}{\sqrt{\lambda_k}} | V^{-1}_{0k} | . \tag{37}$$

3. The relative error due to application of (37) can be estimated by the inequalities:

$$0 < \frac{V_{00}(\vec{r}) - V_{00}(\vec{t}_{opt})}{V_{00}(\vec{r})} < \frac{2}{a^2 - 1} \tag{38}$$

where $\vec{t}_{opt}$ is the point where $V_{00}(\vec{t})$ attains its minimum in Ω_a .

P r o o f. Neglecting the term with factors of the form $\prod_{i=k_1, \ldots, k_p} t_i$ $(p \leq n-2)$ in (19) and dividing the numerator and denominator of (19) by $\prod_{i=1}^{n} \lambda_i t_i$ we obtain for large t_i

$$V_{00}(\vec{t}) \doteq \tilde{V}_{00}(\vec{t}) = \frac{1}{V^{-1}_{00}} \cdot \frac{1 + \sum_{k=1}^{n} V^{-1}_{kk} \frac{1}{\lambda_k t_k}}{1 + \sum_{k=1}^{n} V^{(0)-1}_{kk} \frac{1}{\lambda_k t_k}} \tag{39}$$

The accuracy of this approximation is the better the greater are the t_i so that it is sufficient to compute the estimate (36) for

$$t_i = \frac{a}{n} \frac{V^{-1}_{ii}}{\lambda_i} .$$

Using (31) and (33) to compute all terms in the sum, with respect to r , in the denominater and numerator of (19) we obtain:

$$V_{00}(\vec{t}) = \tilde{V}_{00}(\vec{t})\ \frac{1+\ \omega\ (b)}{1+\omega\ (c)} \tag{40}$$

where

$$\omega(b) = \frac{1}{(b_n+1)\ b_{n-1}} + \dots + \frac{1}{(b_n+1)\ b_{n-1}\dots b_1}$$

and

$$\omega(c) = \frac{1}{(c_n+1)\ c_{n-1}} + \dots + \frac{1}{(c_n+1)\ c_{n-1}\dots c_1} \ .$$

It follows from lemma 3 that:

$$1 < a \leq b_i \leq c_i \qquad i = \overline{1, n} \ . \tag{41}$$

From (40) and (41) we get:

$$0 \leq V_{00}(\vec{t}) - \tilde{V}_{00}(\vec{t}) \leq V_{00}(\vec{t})\ \omega\ (b) \leq$$
$$\leq V_{00}(\vec{t}) \frac{1}{a+1} \sum_{i=1}^{\infty} \frac{1}{a^i} = V_{00}(\vec{t}) \frac{1}{a^2-1} \ . \tag{42}$$

Taking the logarithm of (39) and using the known inequalities:

$$0 \leq x - \ln(1+x) \leq \frac{x^2}{2} \qquad 0 < x < 1$$

we obtain:

$$0 \leq \ln V_{00}^{-1} + \sum_{k=1}^{n} \frac{V_{kk}^{-1} - V_{kk}^{(0)-1}}{\lambda_k t_k} - \ln V_{00}(t) \leq$$
$$\leq \frac{1}{2} \left(\sum_{k=1}^{n} \frac{V_{kk}^{-1}}{\lambda_k t_k} \right)^2 - \frac{1}{2} \left(\sum_{k=1}^{n} \frac{V_{kk}^{(0)-1}}{\lambda_k t_k} \right)^2 \leq \frac{1}{2a^2} \ . \tag{43}$$

From (35), (43) and lemma 2 we obtain:

$$1 \leq \frac{W_{00}(\vec{t})}{\tilde{V}_{00}(\vec{t})} \leq e^{\frac{1}{2a^2}} \tag{44}$$

and from (41) and (44):

$$\frac{|W_{00}(\vec{t}) - V_{00}(\vec{t})|}{V_{00}(\vec{t})} < \max\{ e^{\frac{1}{2a^2}} - 1;\ \frac{1}{a^2-1} \} = \frac{1}{a^2-1} \tag{45}$$

for all $\vec{t} \subset \Omega_a$.

2. Minimizing $\ln W_{00}(\vec{t})$ by the Lagrange method we obtain (37). It follows from (34), that this solution lies in Ω_a.

3. From (45) and the definition of t_{opt} and $\vec{r}$ we obtain:

$$V_{00}(\vec{t}_{opt}) < V_{00}(\vec{r}) < W_{00}(\vec{r}) + \frac{1}{a^2-1} V_{00}(\vec{r}) <$$

$$< W_{00}(\vec{t}_{opt}) + \frac{1}{a^2-1} V_{00}(\vec{r}) < V_{00}(\vec{t}_{opt}) + \frac{1}{a^2-1} V_{00}(\vec{t}_{opt}) +$$

$$+ \frac{1}{a^2-1} V_{00}(\vec{r}) < V_{00}(\vec{t}_{opt}) + \frac{2}{a^2-1} V_{00}(\vec{r}).$$

From these inequalities follow (38).

The theorem is proved.

<u>E x a m p l e.</u> Let us discuss a simple example given in /4/ :

$$\eta_i(\vec{\theta}) = \theta_1 + x_i\theta_2 + x_i^3\theta_3 ; \quad p_i^2 = \frac{1}{x_i} ; \quad \lambda_i = 1 .$$

Let $y_0 = \theta_1$ and $D_{ij} = D_i\delta_{ij}$.

a) Let us plane measurements in two experimental points: x_1, x_2. We obtain from (37):

$$\frac{r_1}{r_2} = \sqrt{\frac{x_2}{x_1}} \; \frac{D_{22} + x_2(x_1+x_2)D_{33}}{D_{22} + x_1(x_1+x_2)D_{33}}$$

b) Measuring in three points x_1, x_2, x_3 which are computed as optimal in /4/ (design without previvous information) we obtain the following ratios of optimal measuring times for $D_1 = D_2 = D_3 = 1$:

$$r_1 : r_2 : r_3 = 0.51 : 0.48 : 0.01$$

whereas in /4/ :

$$r_1 : r_2 : r_3 = 0.84 : 0.12 : 0.04.$$

<u>Continuous planning of experiments</u>

Substituting (37) into (35) we get a formula which is a function of $x_1, \dots, x_n$. Minimizing this function witn respect to the x_i we can obtain the optimal experimental points.

The optimal experimental points can also be obtained in the case of continuous planning /8/. Assuming, that all t_i are equal (all measurements are simultaneous), the optimal experimental points must maximize the absolute value of the derivative:

$$[\frac{d}{dt} \ln V_{00}(t_1 = t, \ldots, t_n = t]_{t=0}.$$

It follows from (19) and (4), that

$$|[\frac{d}{dt} \ln V_{00}(\vec{t})]_{t=0}| = \frac{1}{V_{00}} \sum_{k=1}^{n} \lambda(x_k)[\vec{f}'(x_k) D\vec{f}(x_0)]^2.$$

The measurements should be perfomed in the points $x_1, \ldots, x_n$ given by:

$$\max_{x_1, \ldots, x_n} \sum_{k=1}^{n} \lambda(x_k)[\vec{f}'(x_k) D\vec{f}(x_0)]^2. \qquad (46)$$

The formula (46) is a generalization of (7) in /8/. For $n=1$ (46) coincides with /8/ if one parameter is specified. Some formal differences can be eliminated by simplifying the statement of theorem III in /8/ by means of the lemma 2 of this paper.

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