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CONSTRUCTION METHOD OF A-OPTIMAL CHEMICAL BALANCE WEIGHING DESIGNS

Abstract. In the paper we study the design in which we determine unknown measurements of p objects by use of n measurement operations. For that reason we consider the chemical balance weighing design under the assumption that the measurement errors are uncorrelated and they have the same variances. We give new construction method of the A-optimal chemical balance weighing design based on the incidence matrices of the balanced bipartite weighing designs and the ternary balanced block designs. The consequence of the proposed method is widening of possible classes in which A-optimal design exists**.**

Keywords: A-optimality, balanced bipartite weighing design, chemical balance weighing design, ternary balanced block design

1. INTRODUCTION

Let us consider the linear model

$$\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}, \tag{1}$$

where $\mathbf{y}$ is an $n \times 1$ random vector of observed measurements, $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$, $\mathbf{\Phi}_{n\times p}(-1,0,1)$ denotes the class of $n \times p$ matrices $\mathbf{X} = (x_{ij})$ of elements equal to -1, 1 or 0, $i = 1,2,...,n$, $j = 1,2,...,p$. Any matrix $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ is called the design matrix of the chemical balance weighing design. Moreover, $\mathbf{w}$ is a $p \times 1$ vector representing unknown measurements of objects and $_{e}$ is an $n \times 1$ vector of random errors. We assume that there are no systematic errors, i.e. $\mathrm{E}(\mathbf{e}) = \mathbf{0}_n$ and the errors are non-correlated and they have the same variances, i.e. $\mathrm{Cov}(\mathbf{e}) = \sigma^2\mathbf{I}_n$, where $\mathbf{0}_n$ is vector of zeros, $\sigma > 0$ is known parameter, $\mathbf{I}_n$ denotes identity matrix of rank n.

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For the estimation of $\mathbf{w}$ we use the normal equation $\mathbf{X}'\mathbf{X}\mathbf{w} = \mathbf{X}'\mathbf{y}$. Any chemical balance weighing design $\mathbf{X}$ is nonsingular if and only if the information matrix $\mathbf{M} = \mathbf{X}'\mathbf{X}$ of the design $\mathbf{X}$, is nonsingular. Provided that $\mathbf{X}'\mathbf{X}$ is nonsingular we obtain the least squares estimator of $\mathbf{w}$ given by $\hat{\mathbf{w}} = \left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{X}'\mathbf{y}$ and $\mathrm{Var}(\hat{\mathbf{w}}) = \sigma^2\left(\mathbf{X}'\mathbf{X}\right)^{-1}$.

It is worth noting that the chemical balance weighing design is the name of the plan of experiment described through the model (1). The origin of this name comes from early papers dedicated to experiments determining unknown measurements of objects by weighing them on balance with two pans, called chemical balance. Now, such experimental designs are used as the experimental plans in experiments in which the result of experiment y_i can be described as linear combination of unknown measurements of objects w_j with factors of this combination equal to –1, 0 or 1. The statistical problem is how to determine the estimator of the vector of unknown measurements of objects $\mathbf{w}$ when the observations undergo the model (1). Especially, we are interested in the properties of this estimator. It is expected the mean variance of the estimators attained the lowest bound. Hence, the criterion of the A-optimality is considered.

In the literature many problems concerning weighing experiments are presented. The classical works here are Jacroux *et al.* (1983), Masaro and Wong (2008), Ceranka and Graczyk (2012, 2014b), Katulska and Smaga (2013). Several problems of applications of weighing designs are given in many papers including Banerjee (1975), Graczyk (2013) and Ceranka and Graczyk (2014a). Among several questions taken under consideration, different optimality criteria of the experimental designs are presented. Here, we study the criterion of the A-optimality. Determining A-optimal design we set the design in which the mean variance of the estimators is the smallest. We said that the design $\mathbf{X}_{\mathrm{A}}$ is A-optimal in the class of the designs $\mathbf{\Psi} \subset \mathbf{\Phi}_{n\times p}(-1,0,1)$ if $\mathrm{tr}\left(\mathbf{X}'\mathbf{X}\right)^{-1} = \min\left\{\mathrm{tr}\left(\mathbf{M}^{-1}\right): \mathbf{X} \in \mathbf{\Psi}\right\}$. In the case of the chemical balance weighing designs we obtain the definition given by Ceranka and Graczyk (2007).

Definition 1. Any nonsingular chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ is regular A-optimal if

$$\mathrm{tr}\left(\mathbf{X}'\mathbf{X}\right)^{-1} = p^2(qn)^{-1}, \tag{2}$$

where $q = \max\{q_1, q_2, ..., q_n\}$, $q_i = \sum_{j=1}^{p} x_{ij}^2$, $i = 1,2,...,n.$

In the same paper the condition determining A-optimal design is presented.

Theorem 1. Any nonsingular chemical balance weighing design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}(-1,0,1)$ is regular A-optimal if and only if

$$\mathbf{X}'\mathbf{X} = qnp^{-1}\mathbf{I}_n . \tag{3}$$

In the present paper the construction of the design matrix of the regular A-optimal chemical balance weighing design is based on the incidence matrices of the balanced bipartite weighing designs and the ternary balanced block designs. So, in the next section we present the definitions of the balanced bipartite weighing design and the ternary balanced block design.

2. BALANCED DESIGNS

Any balanced bipartite weighing design there is an arrangement of v treatments into b blocks in such a way that each block containing k distinct treatments is divided into 2 subblocks containing k_1 and k_2 treatments, respectively, where $k = k_1 + k_2$. Each treatment appears in r blocks, each pair of treatments from different subblocks appears together in λ_1 blocks and each pair of treatments from the same subblock appears together in λ_2 blocks. The integers v, b, r, k_1, k_2, λ_1, λ_2 are called the parameters of the balanced bipartite weighing design and satisfy the following equalities $vr = bk$, $b = \lambda_1 v(v-1)(2k_1k_2)^{-1}$, $r = \lambda_1 k(v-1)(2k_1k_2)^{-1}$, $\lambda_2 = \lambda_1(k_1(k_1-1)+k_2(k_2-1))(2k_1k_2)^{-1}$. Let $\mathbf{N}$ be the incidence matrix of such a design with the elements equal to 0 or 1, then $\mathbf{NN}' = (r-\lambda_1-\lambda_2)\mathbf{I}_v + (\lambda_1+\lambda_2)\mathbf{1}_v\mathbf{1}_v'$. For more details we refer the reader to Swamy (1982).

Any ternary balanced block design (see Billington, 1984) is an arrangement of v treatments in b blocks, each of size k in such a way that each treatment appears 0, 1 or 2 times in r blocks. Each of the distinct pairs of treatments appears λ times. Any ternary balanced block design is regular, that is, each treatment occurs alone in ρ_1 blocks and is repeated two times in ρ_2 blocks, where ρ_1 and ρ_2 are constant for the design. It is straightforward to verify that $vr = bk$, $r = \rho_1 + 2\rho_2$, $\lambda(v-1) = \rho_1(k-1) + 2\rho_2(k-2)$. $\mathbf{N}$ is the incidence matrix of such a design with elements equal to 0, 1 or 2, and moreover $\mathbf{NN}' = (\rho_1 + 4\rho_2 - \lambda)\mathbf{I}_v + \lambda\mathbf{1}_v\mathbf{1}_v'$.

3. CONSTRUCTION OF REGULAR A-OPTIMAL DESIGNS

Let $\mathbf{N}$ be the incidence matrix of the balanced bipartite weighing 2design with the parameters v, b_1, r_1, k_{11}, k_{21}, λ_{11}, λ_{21}. From the matrix $\mathbf{N}$ we form the matrix $\mathbf{N}_1$ by replacing k_{11} elements equal to $+1$ of each column which correspond to the elements belonging to the first sub-block by -1. Thus, each column of the matrix $\mathbf{N}_1$ will contain k_{11} elements equal to -1, k_{21} elements equal to $+1$ and $v-k_{11}-k_{21}$ elements equal to 0. Next, let $\mathbf{N}_2$ be the incidence matrix of the ternary balanced block design with the parameters v, b_2, r_2, k_2, λ_2, ρ_{12}, ρ_{22}. From the matrices $\mathbf{N}_1$ and $\mathbf{N}_2$ we construct the design matrix $\mathbf{X}$ of the chemical balance weighing design in the form

$$\mathbf{X}=\begin{bmatrix}\mathbf{N}_1^{'}\\ \mathbf{N}_2^{'}-\mathbf{1}_{b_2}\mathbf{1}_v^{'}\end{bmatrix}. \tag{4}$$

In this design $p=v$ and $n=b_1+b_2$.

Lemma 1. Any chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ in the form (4) is nonsingular if and only if

$$k_{11}\neq k_{12} \tag{5}$$

$$v\neq k_2. \tag{6}$$

Proof. For the matrix $\mathbf{X}$ in (4), we have

$$\mathbf{X}^{'}\mathbf{X}=\left(r_1-\lambda_{21}+\lambda_{11}+r_2+2\rho_{22}-\lambda_2\right)\mathbf{I}_v+\left(\lambda_{21}-\lambda_{11}+b_2-2r_2+\lambda_2\right)\mathbf{1}_v\mathbf{1}_v^{'}. \tag{7}$$

In this way we obtain

$$\det\left(\mathbf{X}^{'}\mathbf{X}\right)=\left(r_1-\lambda_{21}+\lambda_{11}+r_2+2\rho_{22}-\lambda_2\right)^{v-1}\cdot$$

$$\cdot\left(\frac{r_2}{k_2}\left(v-k_2\right)^2+\frac{(v-1)\lambda_{11}}{2k_{11}k_{21}}\left(k_{11}-k_{21}\right)^2\right).$$

The determinant is equal to 0 if and only if $v-k_2=0$ and $k_{11}-k_{12}=0.$ From the above considerations we conclude that the matrix $\mathbf{X}'\mathbf{X}$ is nonsingular if and only if at least one of the conditions (5) and (6) is satisfied, that finishes the proof.

Theorem 2. Any nonsingular chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ given in the form (4) is regular A-optimal if and only if

$$\lambda_{21}-\lambda_{11}+b_2-2r_2+\lambda_2=0 \quad \text{and} \tag{8}$$

$$r_1+b_2-\rho_{12}=q(b_1+b_2)v^{-1}. \tag{9}$$

Proof. As in the proof of Lemma 1, for the matrix $\mathbf{X}$ in (4), the equality (7) is satisfied and what is more the condition (3) holds. Comparing these two equalities we get the equality (8) and $r_1-\lambda_{21}+\lambda_{11}+r_2+2\rho_{22}-\lambda_2=v^{-1}q(b_1+b_2)$. Consequently, under the assumption that the equality (8) is fulfilled, from the last equation we obtain the condition (9). In this way we get the thesis of Theorem.

In particular case, the equality (8) is true when $\lambda_{21}=\lambda_{11}$ and $b_2=2r_2-\lambda_2.$ In this situation we have the following Theorem.

Theorem 3. The existence of the balanced bipartite weighing design with the parameters $v=3s+1,\quad b_1=0.5us(3s+1),\quad r_1=2us,\quad k_{11}=1,\quad k_{21}=3,$ $\lambda_{11}=\lambda_{21}=u$ and the ternary balanced block designs with the parameters $v=3s+1,\ b_2=t(3s+1),\ r_2=t(3s-1),\ k_2=3s-1,\ \lambda_2=\rho_{12}=3t(s-1),\ \rho_{22}=t,$ $s=2,3,\ldots,\ t,u=1,2,\ldots,$ implies the existence of the regular A-optimal chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ in (4).

Proof. It is easy to check that the parameters given above satisfy the conditions (8) and (9).

Theorem 4. The existence of the balanced bipartite weighing design with the parameters $v=s,\quad b_1=0.5us(s-1),\quad r_1=2u(s-1),\quad k_{11}=1,\quad k_{21}=3,$ $\lambda_{11}=\lambda_{21}=3u$ and the ternary balanced block designs with the parameters $v=s,$ $b_2=ts,\quad r_2=t(s-2),\quad k_2=s-2,\quad \lambda_2=\rho_{12}=t(s-4),\quad \rho_{22}=t,\quad s=5,6,\ldots,$ $t,u=1,2,\ldots,$ implies the existence of the regular A-optimal chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ given in the form (4).

Proof. Easy computations show that the parameters given above satisfy the conditions (8) and (9).

Theorem 5. The existence of the balanced bipartite weighing design with the parameters $v=36s+1,\quad b_1=us(36s+1),\quad r_1=9us,\quad k_{11}=3,\quad k_{21}=6,$ $\lambda_{11}=\lambda_{21}=u$ and the ternary balanced block designs with the parameters $v=36s+1,\quad b_2=t(36s+1),\quad r_2=2t(18s-1),\quad k_2=2(18s-1),\quad \lambda_2=t(36s-5),$ $\rho_{12}=4t(9s-2),\quad \rho_{22}=3t,\quad s,t,u=1,2,\ldots,$ implies the existence of the regular A-optimal chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ given in the form (4).

Proof. One can easily prove that the parameters given above satisfy the conditions (8) and (9).

The equality (8) is also satisfied when $\lambda_{21}-\lambda_{11}=\alpha$ and $b_2+\lambda_2-2r_2=-\alpha.$ Hence

Theorem 6. The existence of the balanced bipartite weighing design with the parameters and the ternary balanced block designs with the parameters

i) $v=b_1=5,\ r_1=4,\ k_{11}=k_{21}=\lambda_{11}=2,\ \lambda_{21}=1$ and $v=5,\ b_2=15,\ r_2=9,$ $k_2=3,\ \lambda_2=4,\ \rho_{12}=7,\ \rho_{22}=1,$

ii) $v=b_1=r_1=5,\quad k_{11}=1,\quad k_{21}=4,\quad \lambda_{11}=2,\quad \lambda_{21}=3$ and $v=k_2=5,$ $b_2=r_2=10,\ \lambda_2=9,\ \rho_{12}=6,\ \rho_{22}=2,$

iii) $v=6,\quad b_1=30,\quad r_1=15,\quad k_{11}=1,\quad k_{21}=2,\quad \lambda_{11}=4,\quad \lambda_{21}=2$ and $v=6,$ $b_2=18,\ r_2=9,\ k_2=3,\ \lambda_2=2,\ \rho_{12}=1,\ \rho_{22}=4,$

iv) $v=9,\quad b_1=18,\quad r_1=8,\quad k_{11}=k_{21}=\lambda_{11}=2,\quad \lambda_{21}=1$ and $v=9,\quad b_2=36,$ $r_2=24,\ k_2=6,\ \lambda_2=13,\ \rho_{12}=8,\ \rho_{22}=8,$

v) $v=9,\quad b_1=18,\quad r_1=10,\quad k_{11}=1,\quad k_{21}=4,\quad \lambda_{11}=2,\quad \lambda_{21}=3$ and $v=b_2=r_2=k_2=9,\ \lambda_2=8,\ \rho_{12}=1,\ \rho_{22}=4,$

vi) $v=9,\quad b_1=18,\quad r_1=10,\quad k_{11}=2,\quad k_{21}=\lambda_{11}=3,\quad \lambda_{21}=2$ and $v=9,$ $b_2=18,\ r_2=12,\ k_2=6,\ \lambda_2=7,\ \rho_{12}=8,\ \rho_{22}=2,$

vii) $v=9,\quad b_1=18,\quad r_1=16,\quad k_{11}=2,\quad k_{21}=\lambda_{11}=6,\quad \lambda_{21}=8$ and $v=k_2=9,$ $b_2=r_2=18,\ \lambda_2=\rho_{22}=8,\ \rho_{12}=2,$

viii) $v=9,\quad b_1=36,\quad r_1=12,\quad k_{11}=1,\quad k_{21}=\lambda_{11}=2,\quad \lambda_{21}=1$ and $v=9,\quad b_2=36,$ $r_2=24,\ k_2=6,\ \lambda_2=13,\ \rho_{12}=\rho_{22}=8,$

ix) $v=9,\ b_1=36,\ r_1=28,\ k_{11}=2,\ k_{21}=5,\ \lambda_{11}=10,\ \lambda_{21}=11$ and $v=9,\ b_2=18,\ r_2=18,\ k_2=9,\ \lambda_2=17,\ \rho_{12}=10,\ \rho_{22}=4,$

x) $v=b_1=11,\ r_1=6,\ k_{11}=\lambda_{11}=1,\ k_{21}=5,\ \lambda_{21}=2$ and $v=b_2=$ $=r_2=k_2=11,\ \lambda_2=10,\ \rho_{12}=1,\ \rho_{22}=5,\ v=11,\ b_1=55,\ r_1=35,\ k_{11}=2,\ k_{21}=5,\ \lambda_{11}=10,\ \lambda_{21}=11$ and $v=k_2=11,\ b_2=r_2=44,\ \lambda_2=43,\ \rho_{12}=34,\ \rho_{22}=5,$

xi) $v=13,\ b_1=39,\ r_1=24,\ k_{11}=2,\ k_{21}=\lambda_{11}=6,\ \lambda_{21}=8$ and $v=k_2=13,\ b_2=r_2=30,\ \lambda_2=16,\ \rho_{12}=6,\ \rho_{22}=12,$

xii) $v=15,\ b_1=105,\ r_1=49,\ k_{11}=2,\ k_{21}=5,\ \lambda_{11}=10,\ \lambda_{21}=11$ and $v=k_2=15,\ b_2=r_2=30,\ \lambda_2=29,\ \rho_{12}=16,\ \rho_{22}=7,$

implies the existence of the regular A-optimal chemical balance weighing design $\mathbf{X}\in\mathbf{\Phi}_{n\times p}(-1,0,1)$ given in the form (4).

Proof. We see at once that the parameters given above satisfy the conditions (8) and (9).

4. EXAMPLE

Chemical balance weighing designs can be applied in all experiments in which the experimental factors are on three levels. Let us suppose, we study the real estate market and we are interested in the influence of factors: population density, kind of occupation, salary, family volume and the location (each on three levels coded with –1, 0 and 1). From the statistical point of view, we are interested in determining the influences of these factors using twenty different combinations. In the notation of weighing designs we determine unknown measurements of $p=5$ objects in $n=20$ measurements, so we consider the class $\mathbf{\Phi}_{20\times5}(-1,0,1)$. Based on the Theorem 4 for $s=5,\ u=1$ and $t=2,$ we consider the balanced bipartite weighing design with the parameters $v=5$, $b_1=10,\ r_1=8,\ k_{11}=1,\ k_{21}=3,\ \lambda_{11}=3,\ \lambda_{21}=3$ given by the incidence matrix $\mathbf{N}$. From the matrix $\mathbf{N}$ we form the matrix $\mathbf{N}_1$ as described above. So we obtain $\mathbf{N}=\begin{bmatrix} 0 & 1_2 & 1_2 & 1_2 & 1_1 & 0 & 1_2 & 1_1 & 1_2 & 1_2 \\ 1_1 & 0 & 1_2 & 1_2 & 1_2 & 1_2 & 0 & 1_2 & 1_1 & 1_2 \\ 1_2 & 1_1 & 0 & 1_2 & 1_2 & 1_2 & 1_2 & 0 & 1_2 & 1_1 \\ 1_2 & 1_2 & 1_1 & 0 & 1_2 & 1_1 & 1_2 & 1_2 & 0 & 1_2 \\ 1_2 & 1_2 & 1_2 & 1_1 & 0 & 1_2 & 1_1 & 1_2 & 1_2 & 0 \end{bmatrix}$ and

$$\mathbf{N}_1 = \begin{bmatrix} 0 & 1 & 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 \\ -1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & -1 & 1 \\ 1 & -1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & -1 \\ 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 0 \end{bmatrix}.$$ Next, let us consider the ternary balanced block designs with the parameters $v = 5,\ b_2 = 10,$ $r_2 = 6,\ k_2 = 3,\ \lambda_2 = 2,\ \rho_{12} = 2,\ \rho_{22} = 2$ given by the incidence matrix

$$\mathbf{N}_2 = \begin{bmatrix} 2 & 0 & 0 & 0 & 1 & 2 & 0 & 0 & 1 & 0 \\ 1 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 1 \\ 0 & 1 & 2 & 0 & 0 & 1 & 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 2 & 0 & 0 & 1 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 & 2 & 0 & 0 & 1 & 0 & 2 \end{bmatrix}.$$ Thus we obtain the design $\mathbf{X} \in \mathbf{\Phi}_{20\times 5}(-1,0,1)$ given in the form (4) of the regular A-optimal chemical balance weighing given as

$$\mathbf{X}' = \begin{bmatrix} 0 & 1 & 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 \\ -1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & -1 & 1 & 0 & 1 & -1 & -1 & -1 & -1 & 1 & -1 & -1 & 0 \\ 1 & -1 & 0 & 1 & 1 & 1 & 1 & 0 & 1 & -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 & 1 & -1 & -1 \\ 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 0 & 1 & -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 & 1 & -1 \\ 1 & 1 & 1 & -1 & 0 & 1 & -1 & 1 & 1 & 0 & -1 & -1 & -1 & 0 & 1 & -1 & -1 & 0 & -1 & 1 \end{bmatrix}.$$

5. CONCLUSIONS

In this paper some new methods of construction of regular A-optimal chemical balance weighing designs are presented. They permit determining the experimental plans having required statistical properties for many combinations of p and n which have not been presented in the literature up till now. In theorems 3–6 the series of parameters of the balanced bipartite weighing designs and the ternary balanced block designs are presented. Based on these parameters we form the incidence matrices of respective designs, and next the design matrix $\mathbf{X}$ of the regular A-optimal chemical balance weighing design in the form (4). In the literature different optimality criteria are considered. Here, the criterion of A-optimality is preferable as we obtain estimators with the smallest mean variance.

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METODA KONSTRUKCJI A-OPTYMALNEGO CHEMICZNEGO UKŁADU WAGOWEGO

Streszczenie. W pracy zaprezentowana została problematyka związana z układami A-optymalnymi. Rozważamy układ eksperymentalny, w którym wyznaczamy nieznane miary p obiektów w n operacjach pomiarowych. Nieznane miary obiektów wyznaczamy w chemicznym układzie wagowym przy założeniu, że błędy pomiarów są nieskorelowane i mają równe wariancje. Podajemy nową metodę konstrukcji macierzy A-optymalnego chemicznego układu wagowego. Do konstrukcji wykorzystano macierze incydencji dwudzielnych układów bloków oraz trójkowych zrównoważonych układów bloków. Podana konstrukcja znacznie poszerza klasę układów, w której możliwe jest wyznaczenie układu A-optymalnego.

Słowa kluczowe: chemiczny układ wagowy, dwudzielny układ bloków, trójkowy zrównoważony układ bloków, układ A-optymalny.