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A study of the efficiency of chemical balance weighing designs

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SUMMARY

Some elements concerning the problem of determining chemical balance designs are considered. A method is presented for determining the best design in classes where no D-optimal design exists. In this case, we obtain a design that is highly D-efficient. The efficiency of such a design is presented as a function of the number of parameters and measurements, and its properties are studied. Charts showing the efficiency function for selected classes of designs are presented.

Key words: chemical balance weighing, design plan of experiment, D-optimality

1. Introduction

We consider the class of matrices $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ of known elements equal to -1, 0 or 1. Each element of this class $\mathbf{X} = (x_{ij})$ is called the matrix of a chemical balance weighing design, $i = 1,2,\dots,n$, $j = 1,2,\dots,p$. Let an $n \times 1$ random vector of observations $\mathbf{y}$ be given by the formula $\mathbf{y} = \mathbf{X}\mathbf{w} + \mathbf{e}$, where $\mathbf{w}$ is a $p \times 1$ vector of unknown measurements of objects, $\mathbf{e}$ is an $n \times 1$ random vector of errors with E($\mathbf{e}$)=$\mathbf{0}_n$ and Var($\mathbf{e}$)=$\sigma^2\mathbf{I}_n$, where $\mathbf{0}_n$ is the $n \times 1$ vector with zero elements everywhere, and σ^2 is a constant.

Basic problems related to weighing designs can be found in Jacroux et al. (1983), Sathe and Shenoy (1990), and the references cited therein. Some weighing plans are used in spectroscopy (see Harwit and Sloane, 1979). An important application of weighing designs is 2^n fractional factorial designs; see

Cheng (2014). Cheng and Kao (2015) used these designs in neuroimaging experiments, where functional magnetic resonance imaging (fMRI) technology was used to gain knowledge on how the brain reacts to certain mental stimuli. Another common study of applications of weighing designs is given by Graczyk (2013).

For the estimation of unknown measurements of objects $\mathbf{w}$, we use the normal equations $\mathbf{X}'\mathbf{X}\mathbf{w} = \mathbf{X}'\boldsymbol{y}$. If the matrix $\mathbf{X}$ is of full column rank, then the generalized least squares estimator of $\mathbf{w}$ is given by $\hat{\mathbf{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\boldsymbol{y}$ and $\mathrm{Var}(\widehat{\mathbf{w}}) = \sigma^2(\mathbf{X}'\mathbf{X})^{-1}$. The matrix $\mathbf{M} = \mathbf{X}'\mathbf{X}$ is called the information matrix for the design. Some problems relating to criteria for the optimality of chemical balance weighing designs are considered in the literature; see Sathe and Shenoy (1990), Masaro and Wong (2008), Neubauer and Pace (2010), Katulska and Smaga (2013), Smaga (2014), Ceranka and Graczyk (2020a,b). These criteria minimize certain functions of the information matrix $\mathbf{M}$.

In the present paper, we consider D-optimal designs, i.e. optimal in the sense of minimizing the generalized variance of parameter estimates. The design $\mathbf{X}_\mathrm{D}$ is called D-optimal in the given class $\boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$ if $\det\left(\mathbf{X}_\mathrm{D}'\mathbf{X}_\mathrm{D}\right) = max\left\{\det(\mathbf{M}^{-1}) : \mathbf{X} \in \boldsymbol{\Phi}_{n\times p}\{-1,0,1\}\right\}$. If $\det(\mathbf{M}^{-1})$ attains the upper bound, then the design is called regular D-optimal. In other cases, such a design is called D-optimal. Every regular D-optimal design is D-optimal, but the converse may not hold. The limits of functions of the information matrix $\mathbf{M}$ are presented in the literature, for example by Ceranka and Graczyk (2009).

Many theoretical works provide knowledge to guide the selection of optimal designs; see, for example, Ceranka and Graczyk (2017a,b, 2018). Nevertheless, for any combination of a number of objects and number of measurements, we are unable to determine a regular D-optimal design using the construction methods given in the literature, for example in Ceranka and Graczyk (2014, 2015). For this reason, we present here a new method for the construction.

Because it is not possible to determine a D-optimal design for every class $\boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$, the idea of the present study is to solve the problem in the fixed class $\boldsymbol{\Phi}_{n\times p}\{-1,0,1\}$. In our solution we propose to determine a D-optimal design in the class $\mathbf{\Phi}_{(n-s)\times p}\{-1,0,1\}, s = 1,2,3,4$, and then add measurements so that in the initial class we obtain a design with the highest possible efficiency. The efficiency coefficient is determined by the formula given by Bulutoglu and Ryan (2009):

$$\mathrm{D_{eff}}(\mathbf{X}) = \left(\frac{\det(\mathbf{X}'\mathbf{X})}{\det(\mathbf{X}'_{\mathrm{D}}\mathbf{X}_{\mathrm{D}})}\right)^{1/p} \tag{1}$$

where $\mathbf{X}_{\mathrm{D}}$ is a regular D-optimal design. Such a method was presented in Graczyk and Ceranka (2017a).

2. Study of efficiency

In order to indicate a design with the highest possible efficiency in the fixed class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ let us consider the design $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ in the form

$$\mathbf{X} = \begin{bmatrix} \mathbf{X}_s \\ \boldsymbol{x}'_1 \\ \vdots \\ \boldsymbol{x}'_s \end{bmatrix} \tag{2}$$

where

(i) $\mathbf{X}_s \in \mathbf{\Phi}_{(n-s)\times p}\{-1,0,1\}$ is the design matrix of a regular D-optimal chemical balance weighing design,

(ii) $\boldsymbol{x}_h$ are any $p \times 1$ vectors of elements $-1, 0$ or 1, $\boldsymbol{x}'_h\boldsymbol{x}_h = t_h$, $\boldsymbol{x}'_h\boldsymbol{x}_{h'} = \boldsymbol{x}'_{h'}\boldsymbol{x}_h = u_{hh'}$,

(iii) $s = 1,2,3,4$, $h, h' = 1,2,\dots,s$, $h \neq h'$, $1 \leq t_h \leq p$.

Our goal now is to investigate the properties of $\mathrm{D_{eff}}(\mathbf{X})$ for any $\mathbf{X} \in \mathbf{\Phi}_{n\times p}\{-1,0,1\}$ for $s = 1,2,3,4$, depending on the number of objects p and the maximal number m of elements equal to –1 or 1 in columns of $\mathbf{X}$. According to the formula (1) and the considerations given by Ceranka and Graczyk (2017a), the efficiency of any chemical balance weighing design of the form (2) is given by the formula

$$\mathrm{D_{eff}}(\mathbf{X}) = \frac{m}{m+s} \cdot \sqrt[p]{\frac{(m+p)^s}{m^s} - \tau_\xi}, \tag{3}$$

where τ_ξ is as given in Table 1.

Table 1. The value of τ_ξ in (3) determined for a fixed value of the number of objects p and the number of additional measurements s.

τ_ξ	s	p
0	1	
0	2	$p \equiv 0 \ (mod\ 2)$
m^{-s}	2	$p \equiv 1 \ (mod\ 2)$
0	3,4	$p \equiv 0 \ (mod\ 4)$
$\frac{3(s-2)(m+p)^{s-2} - 2^{s-1}(s-3)(m+p) - (s-1)}{m^s}$	3,4	$p+1 \equiv 0 \ (mod\ 4)$
$\frac{3(s-2)(m+p)^{s-2} + 2^{s-1}(s-3)(m+p) - (s-1)}{m^s}$	3,4	$p+3 \equiv 0 \ (mod\ 4)$
$\frac{4^{s-2}(m+p)^{s-2} + 4(s-3)}{m^s}$	3,4	$p+2 \equiv 0 \ (mod\ 4)$

Theorem 1. $\mathrm{D_{eff}}(\mathbf{X})$ as given by formula (3) and Table 1 is a decreasing function of the variable p for fixed m and s.

Proof. Let us consider the case $s = 1$. For any number of objects p, $\tau_\xi = 0$ and $\mathrm{D_{eff}}(\mathbf{X}) = \frac{m}{m+s} \cdot \sqrt[p]{\frac{(m+p)^s}{m^s}}$. Thus, we obtain $\mathrm{D_{eff}}'(\mathbf{X}) = \frac{m}{m+s} \cdot exp\left\{\frac{s}{p} ln \frac{m+p}{m}\right\} \cdot \frac{s}{p^2}\left(\frac{p}{p+m} - ln\frac{m+p}{m}\right)$. We set $\mathrm{D_{eff}}'(\mathbf{X}) = \frac{m}{m+s} \cdot exp\left\{\frac{s}{p} ln\frac{m+p}{m}\right\} \cdot \frac{s}{p^2} \cdot g(\tau)$ where $\tau = \frac{p}{m}$, $g(\tau) = \frac{\tau}{1+\tau} - \ln(1+\tau)$. We study the function $g(\tau)$. Note that $g(0) = 0$ and $g'(\tau) = -\tau(1+\tau)^{-2} < 0$. Since $g(0) = 0$ and the function $g(\tau)$ is decreasing, we have $\frac{\tau}{1+\tau} < \ln(1+\tau)$. The proof for other values of s is analogous.

Let us consider the formula (3) for different values of p and m, i.e. the number of objects and the maximal number of elements equal to -1 or 1 in columns of $\mathbf{X}$. In Tables 2–5 and Figures 1–4 we present the values of $\mathrm{D_{eff}}(\mathbf{X})$ for $p \leq 20$ and $m \leq 10$.

Table 2. Values of $\mathrm{D_{eff}}(\mathrm{X})$ for given p and m with one additional measurement

	m									
p	1	2	3	4	5	6	7	8	9	10
3	0.7937	0.9048	0.9449	0.9640	0.9746	0.9811	0.9854	0.9884	0.9906	0.9922
4	0.7476	0.8773	0.9269	0.9513	0.9652	0.9739	0.9796	0.9837	0.9866	0.9898
5	0.7154	0.8564	0.9125	0.9408	0.9572	0.9676	0.9745	0.9795	0.9831	0.9858
6	0.6915	0.8399	0.9007	0.9319	0.9503	0.9621	0.9700	0.9758	0.9800	0.9832
7	0.6729	0.8264	0.8990	0.9243	0.9443	0.9572	0.9660	0.9724	0.9774	0.9807
8	0.6580	0.8152	0.8822	0.9177	0.9390	0.9529	0.9624	0.9693	0.9744	0.9784
9	0.6457	0.8056	0.8748	0.9119	0.9343	0.9490	0.9591	0.9665	0.9720	0.9762
10	0.6354	0.7974	0.8684	0.9067	0.9301	0.9454	0.9561	0.9640	0.9698	0.9743
11	0.6267	0.7903	0.8627	0.9021	0.9262	0.9422	0.9534	0.9616	0.9677	0.9725
12	0.6191	0.7840	0.8576	0.8979	0.9228	0.9393	0.9509	0.9594	0.9658	0.9708
13	0.6125	0.7784	0.8530	0.8941	0.9196	0.9366	0.9486	0.9574	0.9641	0.9678
14	0.6067	0.7734	0.8489	0.8907	0.9167	0.9341	0.9464	0.9555	0.9624	0.9664
15	0.6015	0.7689	0.8452	0.8876	0.9140	0.9318	0.9444	0.9537	0.9608	0.9656
16	0.5969	0.7648	0.8417	0.8846	0.9115	0.9296	0.9425	0.9520	0.9593	0.9638
17	0.5927	0.7611	0.8385	0.8820	0.9092	0.9276	0.9408	0.9505	0.9580	0.9629
18	0.5889	0.7576	0.8356	0.8795	0.9071	0.9258	0.9391	0.9490	0.9566	0.9626
19	0.5854	0.7545	0.8329	0.8771	0.9051	0.9240	0.9376	0.9477	0.9554	0.9615
20	0.5822	0.7516	0.8304	0.8750	0.9032	0.9223	0.9361	0.9463	0.9542	0.9604

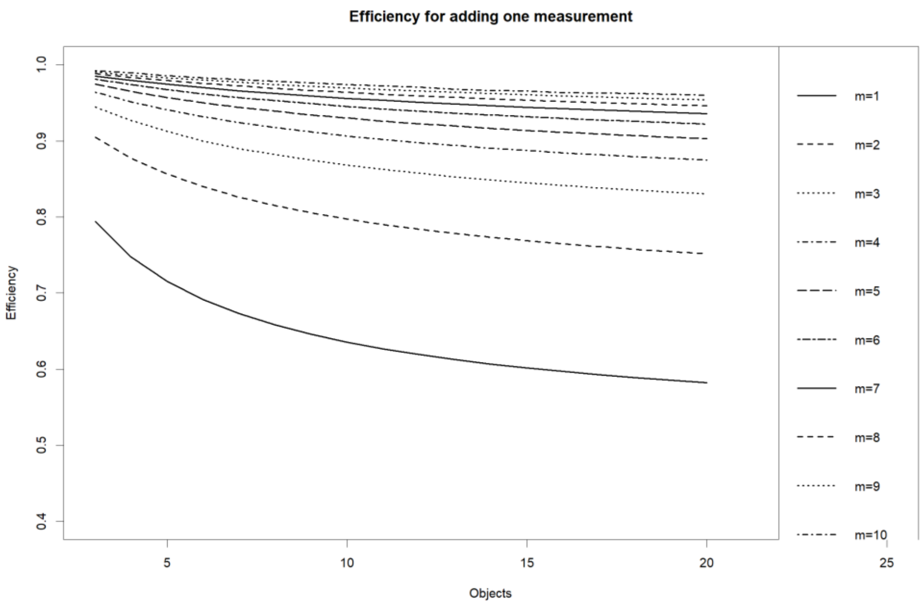

Figure 1. Values of $\mathrm{D_{eff}}(\mathrm{X})$ for given p and m with one additional measurement

Table 3. Values of $\mathrm{D_{eff}}(\mathrm{X})$ for given p and m with two additional measurements

	m									
p	1	2	3	4	5	6	7	8	9	10
3	0.8220	0.9085	0.9435	0.9515	0.9720	0.9787	0.9832	0.9865	0.9889	0.9907
4	0.7453	0.8660	0.9165	0.9428	0.9583	0.9682	0.9749	0.9797	0.9832	0.9860
5	0.6787	0.8218	0.8854	0.9198	0.9406	0.9541	0.9635	0.9703	0.9753	0.9791
6	0.6376	0.7937	0.8653	0.9048	0.9289	0.9449	0.9560	0.9641	0.9701	0.9747
7	0.6024	0.7670	0.8451	0.8890	0.9163	0.9334	0.9474	0.9568	0.9638	0.9693
8	0.5773	0.7476	0.8302	0.8773	0.9070	0.9269	0.9410	0.9513	0.9591	0.9652
9	0.5554	0.7296	0.8158	0.8657	0.8974	0.9189	0.9342	0.9455	0.9541	0.9607
10	0.5384	0.7154	0.8044	0.8564	0.8898	0.9125	0.9288	0.9409	0.9501	0.9572
11	0.5233	0.7023	0.7935	0.8474	0.8821	0.9060	0.9232	0.9360	0.9458	0.9535
12	0.5111	0.6915	0.7845	0.8399	0.8758	0.9007	0.9186	0.9319	0.9422	0.9503
13	0.500	0.6814	0.7760	0.8326	0.8696	0.8953	0.9139	0.9279	0.9386	0.9471
14	0.4907	0.6729	0.7687	0.8264	0.8643	0.8908	0.9099	0.9244	0.9355	0.9444
15	0.4823	0.6650	0.7618	0.8205	0.8592	0.8862	0.9060	0.9208	0.9324	0.9415
16	0.4749	0.6580	0.7557	0.8152	0.8546	0.8822	0.9048	0.9177	0.9296	0.9390
17	0.4683	0.6515	0.7499	0.8102	0.8502	0.8784	0.8990	0.9147	0.9269	0.9366
18	0.4623	0.6458	0.7448	0.8057	0.8463	0.8749	0.8959	0.9119	0.9244	0.9343
19	0.4568	0.6403	0.7399	0.8014	0.8424	0.8715	0.8929	0.9092	0.9219	0.9321
20	0.4520	0.6355	0.7356	0.7975	0.8390	0.8684	0.8902	0.9068	0.9177	0.9301

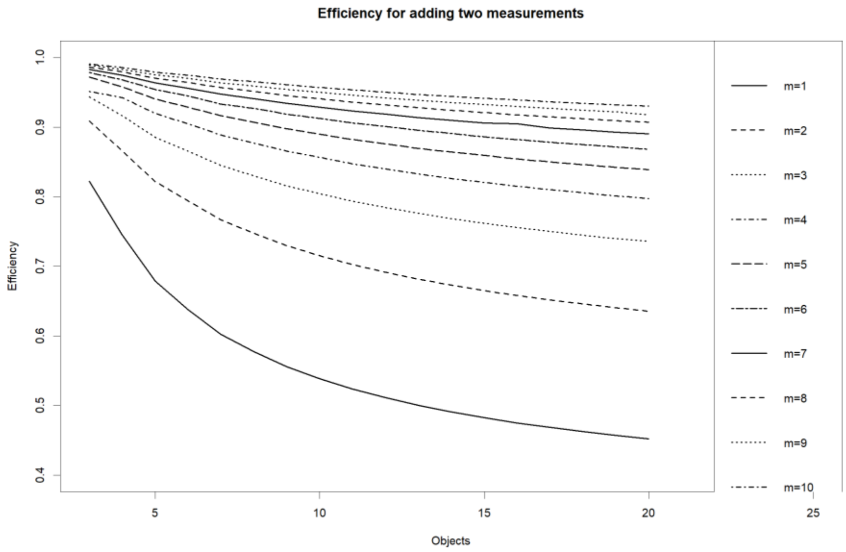

Figure 2. Values **of $\mathbf{D_{eff}}$**(X) for given p and m with two additional measurements

Table 4. Values of $\mathrm{D_{eff}}(\mathrm{X})$ for given p and m with three additional measurements

	m									
p	1	2	3	4	5	6	7	8	9	10
3	0.9210	0.9524	0.9681	0.9771	0.9828	0.9865	0.9892	0.9910	0.9926	0.9937
4	0.8359	0.9118	0.9439	0.9610	0.9712	0.9779	0.9824	0.9857	0.9881	0.9900
5	0.7213	0.8385	0.8927	0.9230	0.9419	0.9589	0.9634	0.9699	0.9748	0.9785
6	0.6521	0.7914	0.8587	0.8973	0.9218	0.9383	0.9501	0.9588	0.9654	0.9705
7	0.6049	0.7576	0.8337	0.8782	0.9065	0.9260	0.9339	0.9502	0.9581	0.9642
8	0.5698	0.7314	0.8113	0.8627	0.8943	0.9160	0.9316	0.9431	0.9520	0.9589
9	0.5369	0.7042	0.7919	0.8448	0.8794	0.9035	0.9209	0.9339	0.9440	0.9518
10	0.5115	0.6827	0.7744	0.8303	0.8674	0.8933	0.9122	0.9264	0.9374	0.9461
11	0.4913	0.6653	0.7599	0.8183	0.8573	0.8847	0.9048	0.9200	0.9318	0.9411
12	0.4747	0.6506	0.7476	0.8081	0.8486	0.8773	0.8984	0.9114	0.9269	0.9368
13	0.4591	0.6361	0.7351	0.7913	0.8393	0.8692	0.8914	0.9082	0.9214	0.9319
14	0.4460	0.6238	0.7243	0.7880	0.8313	0.8623	0.8852	0.9028	0.9165	0.9275
15	0.4349	0.6132	0.7150	0.7799	0.8243	0.8561	0.8798	0.8980	0.9112	0.9236
16	0.4252	0.6039	0.7067	0.7727	0.8179	0.8505	0.8749	0.8936	0.9083	0.9201
17	0.4161	0.5948	0.6985	0.7654	0.8115	0.8448	0.8698	0.8890	0.9042	0.9164
18	0.4081	0.5868	0.6912	0.7588	0.8057	0.8396	0.8651	0.8848	0.9004	0.9130
19	0.4010	0.5796	0.6846	0.7530	0.8004	0.8349	0.8609	0.8811	0.8970	0.9099
20	0.3947	0.5732	0.6787	0.7436	0.7957	0.8307	0.8571	0.8776	0.8939	0.9070

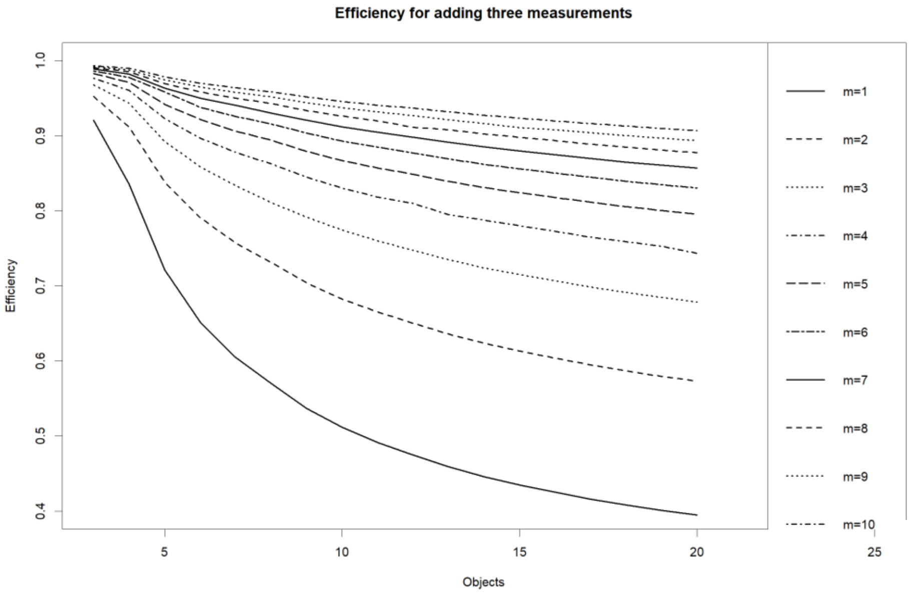

Figure 3. Values of $\mathrm{D_{eff}}(\mathrm{X})$ for given p and m with three additional measurements

Table 5. Values of $\mathrm{D_{eff}}(\mathrm{X})$ for given p and m with four additional measurements

	m									
p	1	2	3	4	5	6	7	8	9	10
3	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
4	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
5	0.8154	0.8890	0.9239	0.9440	0.9569	0.9657	0.9720	0.9767	0.9803	0.9831
6	0.7130	0.8220	0.8765	0.9085	0.9292	0.9435	0.9538	0.9615	0.9674	0.9720
7	0.6454	0.7773	0.8441	0.8840	0.9099	0.9280	0.9410	0.9508	0.9583	0.9642
8	0.6000	0.7453	0.8206	0.8660	0.8958	0.9165	0.9315	0.9428	0.9514	0.9583
9	0.5532	0.7075	0.7902	0.8412	0.8751	0.8991	0.9106	0.9299	0.9402	0.9484
10	0.5184	0.6787	0.7667	0.8221	0.8590	0.8854	0.9049	0.9188	0.9313	0.9406
11	0.4916	0.6559	0.7481	0.8063	0.8460	0.8744	0.8954	0.9116	0.9242	0.9343
12	0.4702	0.6376	0.7328	0.7937	0.8353	0.8653	0.8876	0.9048	0.9182	0.9289
13	0.4495	0.6184	0.7161	0.7747	0.8228	0.8544	0.8781	0.8963	0.9111	0.9222
14	0.4324	0.6024	0.7020	0.7670	0.8122	0.8451	0.8699	0.8890	0.9042	0.9164
15	0.4182	0.5889	0.6902	0.7657	0.8032	0.8372	0.8629	0.8828	0.8986	0.9114
16	0.4061	0.5773	0.6798	0.7476	0.7953	0.8302	0.8567	0.8773	0.8937	0.9070
17	0.3944	0.5656	0.6692	0.7381	0.7867	0.8226	0.8499	0.8712	0.8882	0.9019
18	0.3843	0.5554	0.6598	0.7296	0.7792	0.8158	0.8438	0.8657	0.8832	0.8974
19	0.3755	0.5464	0.6515	0.7221	0.7725	0.8098	0.8384	0.8608	0.8788	0.8934
20	0.3677	0.5385	0.6441	0.7155	0.7665	0.8054	0.8336	0.8565	0.8748	0.8898

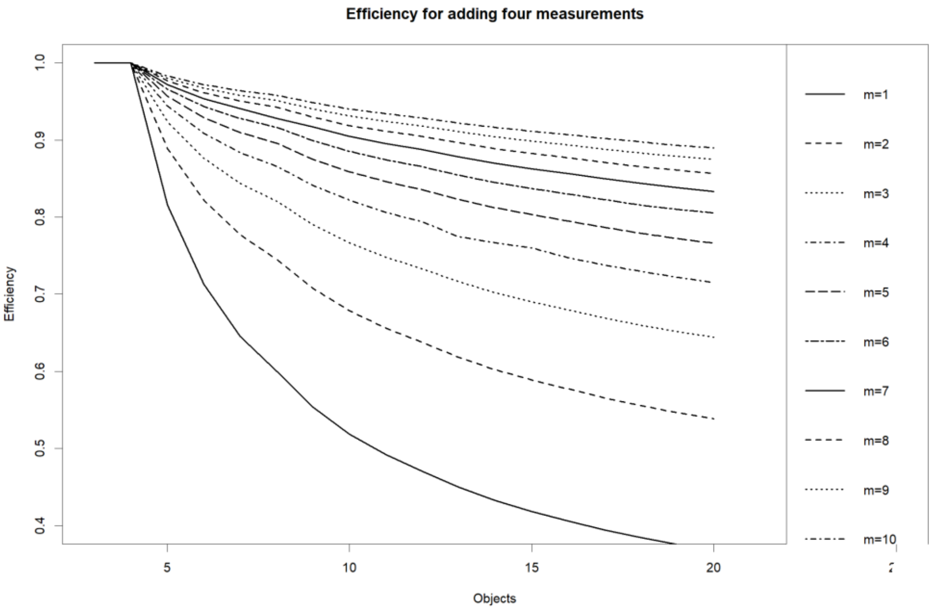

Figure 4. Values of $\mathrm{D_{eff}}(\mathbf{X})$ for given p and m with four additional measurements

3. Discussion

The results presented in this paper make a key contribution to the development of knowledge regarding the planning of experiments using chemical balance weighing designs. Since not for every possible combination of a number of objects and a number of measurements – in other words, not in every class $\mathbf{\Phi}_{n\times p}\{-1,0,1\}$ – can we determine an optimal design, there is a need to indicate which of the possible designs considered will be the best in the class. Hence the need to identify the best design, i.e., the one for which the defined efficiency coefficient will be closest to a value of 1.

The research presented here proposes a solution to this problem based on the consideration of a design in which further measurements are added to the matrix of a design that is optimal in a class for a smaller number of measurements, in such a way that the resulting design has the highest possible efficiency, but now in the initial class.

The studies carried out enable one to make a selection of a design that will be the best (most effective) in the given class, and then, based on the methods presented in Graczyk and Ceranka (2020a,b) to indicate the methods of construction of this system.

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