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ON HIGHLY D-EFFICIENT DESIGNS WITH NON-NEGATIVELY CORRELATED OBSERVATIONS

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Abstract:

- In the most difficult case where the number of observations $n \equiv 3 \pmod 4$, high D-efficiency of certain chemical balance weighing designs under completely symmetric covariance matrix of errors is shown. It is also proved that D-optimal design may depend on the values of the correlation coefficient.

Key-Words:

- *chemical balance weighing design; correlated observations; D-efficiency; D-optimality; Hadamard matrix; simulated annealing algorithm.*

AMS Subject Classification:

- 62K05, 05B20.

1. INTRODUCTION

Let us introduce a model of the chemical balance weighing design. Assume that $\mathcal{M}_{n\times p}(\{-1,1\})$ denotes the set of $n\times p$ matrices whose entries are all equal to 1 or -1. A linear model of the chemical balance weighing design is as follows: $\mathbf{y}=\mathbf{X}\mathbf{b}+\mathbf{e}$, where $\mathbf{y}=(y_1,...,y_n)'$ is a vector of observations, $\mathbf{X}=(x_{ij})\in\mathcal{M}_{n\times p}(\{-1,1\})$ is a design matrix of full column rank ($n\geqslant p$), $\mathbf{b}=(b_1,...,b_p)'$ is a vector of unknown parameters, and $\mathbf{e}=(e_1,...,e_n)'$ is a vector of errors. In a chemical balance, if the j-th object is placed on the left (resp. right) pan during the i-th weighing operation, then $x_{ij}=-1$ (resp. $x_{ij}=1$). Moreover, suppose that $\mathrm{E}(e_i)=0$, $i=1,...,n$ and $\mathrm{Cov}(\mathbf{e})=\sigma^2\mathbf{G}$, where $\sigma>0$ is an unknown parameter and $\mathbf{G}$ is a known positive definite matrix of size n.

Among all designs in $\mathcal{M}_{n\times p}(\{-1,1\})$, we would like to find the optimal design with respect to certain criterion. Optimal weighing designs depend significantly on the form of $\mathbf{G}$. In the literature, optimal weighing designs are mostly considered under the following forms of $\mathbf{G}$: the identity matrix (the errors are uncorrelated and have equal variances; see Banerjee, 1975; Cheng, 2014; Ehlich, 1964; Galil and Kiefer, 1980; Neubauer and Pace, 2010), the diagonal matrix (the errors are uncorrelated and may have different variances; see Ceranka *et al.*, 2006; Graczyk, 2011, 2012), the completely symmetric matrix (the errors are equally correlated and have equal variances; see Ceranka and Graczyk, 2011, 2015; Katulska and Smaga, under review; Masaro and Wong, 2008a, 2008b, 2008c; Smaga, 2015), and the covariance matrix of an AR(1) process (see Angelis *et al.*, 2001; Katulska and Smaga, 2012, 2013; Li and Yang, 2005; Smaga, 2014; Yeh and Lo Huang, 2005). Some applications of optimal weighing designs and real data examples of their use can be found in Banerjee (1975), Cheng (2014), Graczyk (2013) and Jenkins and Chanmugam (1962).

In this paper we consider D-efficiency of chemical balance weighing designs, when the errors are equally correlated and have equal variances. Under this assumption, the matrix $\mathbf{G}$ is of the form:

$$\mathbf{G} = (1-\rho)\,\mathbf{I}_n + \rho\,\mathbf{1}_n\mathbf{1}_n' , \tag{1.1}$$

where $\rho\in[0,1)$ is a known parameter, $\mathbf{I}_n$ is the n-dimensional unit matrix, and $\mathbf{1}_n$ is the n-dimensional column vector of ones. For given ρ, the matrix $\mathbf{G}$ is positive definite and $\mathbf{G}^{-1}=c(\mathbf{I}_n-r\,\mathbf{1}_n\mathbf{1}_n')$, where $c=1/(1-\rho)$ and

$$r = \frac{\rho}{1+(n-1)\,\rho} . \tag{1.2}$$

Following the definition of Bulutoglu and Ryan (2009), the D-efficiency of a design $\mathbf{X}\in\mathcal{M}_{n\times p}(\{-1,1\})$ is given by the formula

$$\text{D-eff}(\mathbf{X}) = \left[\frac{\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})}{\max_{\mathbf{Y}\in\mathcal{M}_{n\times p}(\{-1,1\})}\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y})}\right]^{1/p} .$$

If D-eff$(\mathbf{X}) = 1$, then $\mathbf{X}$ is D-optimal. Unfortunately, the denominator of D-eff$(\mathbf{X})$ is usually not known, and hence we can not calculate D-efficiency of designs. However, Katulska and Smaga (under review) established the lower bound for D-efficiency of a design $\mathbf{X}$ given by

$$\mathrm{D}^*\text{-eff}(\mathbf{X}) \;=\; \frac{\Big[\det\big(\mathbf{X}'(\mathbf{I}_n - r\,\mathbf{1}_n\mathbf{1}_n')\,\mathbf{X}\big)\Big]^{1/p}}{n}\,,$$

where r is as in (1.2), and they used it to show that designs constructed by Masaro and Wong (2008a) and certain other designs are highly D-efficient for many values of design parameters namely n, p and ρ. Nevertheless, they did not consider the most difficult case $n \equiv 3 \pmod 4$, which is different of the others. In the present paper, this case is of interest to us.

The remainder of this paper is organized as follows. In Section 2, we show that certain design constructed by Masaro and Wong (2008a) is highly D-efficient, when the number of observations $n \equiv 3 \pmod 4$ and it is appropriately large or appropriately larger than the number of objects. Section 3 contains simulation study, which suggests that design is D-optimal in many cases, but also indicates situations where are D-better designs than it. A special case, where different designs are D-optimal for different values of ρ, is presented in Section 4. The paper is concluded in Section 5.

2. D-EFFICIENT DESIGNS WHEN $\mathbf{n \equiv 3}$ (mod 4)

Assume that $n \equiv 3 \pmod 4$, $\rho \in [0, 1)$ and $\mathbf{H}_{n+1}$ is a normalized Hadamard matrix of order $n + 1$, i.e. all entries of its first row and first column are all equal to one. Let $\mathbf{W}$ be a matrix received by deleting the first row and column of $\mathbf{H}_{n+1}$. We form a design $\mathbf{L}$ from p columns of $\mathbf{W}$. From the results of Ehlich (1964) and Galil and Kiefer (1980), the design $\mathbf{L}$ is D-optimal in $\mathcal{M}_{n\times p}(\{-1, 1\})$, when $\rho = 0$ and $n \geqslant 2p - 5$. Masaro and Wong (2008a) proved that the design $\mathbf{L}$ is D-optimal for all $\rho > 0$ in

$$\mathcal{D}_3 \;=\; \Big\{\mathbf{X} \in \mathcal{M}_{n\times p}(\{-1, 1\})\colon\, \mathbf{X}'\mathbf{X} = (n+1)\,\mathbf{I}_p - \mathbf{1}_p\mathbf{1}_p'\Big\}\,.$$

But, if $n < 2p - 5$, then $\mathbf{L}$ may not be D-optimal when $\rho = 0$, and hence we can conclude that the similar situation may have place when $\rho > 0$. As we shall see in the next sections, that conjecture seems to be true and the result of Masaro and Wong (2008a) can not be extended from the subclass $\mathcal{D}_3$ to the class $\mathcal{M}_{n\times p}(\{-1, 1\})$. However, we show that the design $\mathbf{L}$ is highly D-efficient in many cases.

The design $\mathbf{L}$ has the following properties $\mathbf{L}'\mathbf{L} = (n+1)\mathbf{I}_p - \mathbf{1}_p\mathbf{1}_p'$ and $\mathbf{L}'\mathbf{1}_n = -\mathbf{1}_p$. The matrix $\mathbf{L}'(\mathbf{I}_n - r\,\mathbf{1}_n\mathbf{1}_n')\mathbf{L}$ has eigenvalues $n+1$ and $n+1-(1+r)p$ with multiplicities $p-1$ and 1 respectively. Hence

$$\text{D}^*\text{-eff}(\mathbf{L}) \;=\; \frac{n+1}{n}\left[\frac{n-p+1-pr}{n+1}\right]^{1/p}, \tag{2.1}$$

where r is given in (1.2). The lower bounds for D*-eff$(\mathbf{L})$ are given in the following theorem.

Theorem 2.1. *Let* $n \equiv 3 \pmod 4$, $n \geqslant 7$, $p = 2, ..., n-1$, $\rho \in (0,1)$ *and* $\text{Cov}(\mathbf{e}) = \sigma^2\mathbf{G}$, *where* $\mathbf{G}$ *is given by* (1.1). *Then,* D*-eff$(\mathbf{L})$ *decreases, when* ρ *increases, and* D*-eff$(\mathbf{L}) > 0.82$. *Moreover, if* $p \leqslant (n-1)/2;\ n-3;\ n-2$, *then* D*-eff$(\mathbf{L}) > 0.93; 0.92; 0.88$, *respectively.*

Proof: Observe that r is an increasing function of ρ. Hence, D*-eff$(\mathbf{L})$ decreases, when ρ increases, which implies

$$\text{D}^*\text{-eff}(\mathbf{L}) \;>\; \frac{n+1}{n}\left[\frac{n-p}{n}\right]^{1/p}$$

(the right hand side of (2.1) as $\rho \to 1$). The derivative of the function f, $f\colon (1,n) \to \mathbb{R}$ defined by $f(x) = \big[(n-x)/n\big]^{1/x}$ is

$$f'(x) \;=\; -\big[(n-x)/n\big]^{1/x}\, x\big((n/x-1)\,\log(1-x/n)+1\big)\big/\big(x^2(n-x)\big)\,.$$

Consider the function g, $g\colon (1,\infty) \to \mathbb{R}$ given by $g(x) = (x-1)\log(1-1/x)+1$. It is easy to calculate that $g'(x) = 1/x + \log(1-1/x)$, $\lim_{x\to\infty} g'(x) = 0$ and $g''(x) = 1/\big((x-1)\,x^2\big)$. Thus, g is decreasing. So $g(x) > 0$, because $\lim_{x\to\infty} g(x) = 0$. Since $n/x > 1$ for all $x \in (1,n)$, it follows that $f'(x) < 0$. So,

$$\text{D}^*\text{-eff}(\mathbf{L}) \;>\; \frac{n+1}{n}\,f(n-1) \;=\; (n+1)\left[\frac{1}{n}\right]^{n/(n-1)}.$$

The function h, $h\colon (6,\infty) \to \mathbb{R}$ is defined by $h(x) = (x+1)\,[1/x]^{x/(x-1)}$. Its derivative is equal to

$$h'(x) \;=\; -\frac{[1/x]^{x/(x-1)}\big(2(x-1)+(x+1)\,\log(1/x)\big)}{(x-1)^2}\,.$$

If $h_1(x) = 2(x-1)+(x+1)\log(1/x)$, then $h_1'(x) = 1-1/x+\log(1/x)$ and $h_1''(x) = (1-x)/x^2 < 0$. Hence, since $h_1'(6)$ is negative, $h_1'(x) < 0$ for all $x > 6$. So, h_1 is decreasing, and $h_1(6) < 0$, which imply $h_1(x) < 0$. Thus, $h'(x) > 0$ and h is increasing. Hence, we conclude that D*-eff$(\mathbf{L})$ is greater than $h(7) = 0.8263$. In a similar way, we can prove the rest of the claim. □

Theorem 2.1 and the examples (see Table 1) imply **L** is a design with high D-efficiency, when n is appropriately large or appropriately larger than p. From the examples, we conclude that, when ρ increases, the decrease of D*-eff(**L**) can be at most a few percent (see Table 1). As p increases, the decrease of D*-eff(**L**) can be quite large, but when n increases, it decreases. Moreover, the lower bound for D-efficiency of **L** increases, when n increases. From the examples, we also observe that D*-eff(**L**) is often much greater than the lower bounds for it obtained in Theorem 2.1.

Table 1: The lower bound for D-efficiency of design **L**.

ρ	n, p							
	$11, 2$	$11, 10$	$15, 2$	$15, 14$	$19, 2$	$19, 18$	$103, 2$	$103, 102$
0	0.9958	0.9119	0.9977	0.9194	0.9986	0.9262	0.9999	0.9713
0.01	0.9949	0.9077	0.9971	0.9152	0.9981	0.9221	0.9999	0.9685
0.1	0.9908	0.8860	0.9948	0.8970	0.9966	0.9064	0.9998	0.9655
0.2	0.9891	0.8757	0.9940	0.8897	0.9961	0.9010	0.9998	0.9651
0.3	0.9883	0.8700	0.9936	0.8860	0.9960	0.8984	0.9998	0.9650
0.4	0.9878	0.8665	0.9934	0.8838	0.9959	0.8969	0.9998	0.9649
0.5	0.9875	0.8641	0.9933	0.8824	0.9958	0.8959	0.9998	0.9649
0.6	0.9872	0.8623	0.9932	0.8813	0.9957	0.8952	0.9998	0.9649
0.7	0.9871	0.8609	0.9931	0.8805	0.9957	0.8947	0.9998	0.9648
0.8	0.9869	0.8598	0.9930	0.8799	0.9957	0.8943	0.9998	0.9648
0.9	0.9868	0.8590	0.9930	0.8794	0.9957	0.8940	0.9998	0.9648
0.99	0.9867	0.8583	0.9930	0.8791	0.9956	0.8938	0.9998	0.9648

3. SIMULATIONS

In this section we compare the design **L** with the best designs found by simulated annealing algorithm (SA algorithm) proposed by Angelis *et al.* (2001). It is an algorithm for searching optimal designs with very good performance. The SA algorithm was executed at least 1000 times for many values of n, p and ρ. The initial parameters of this algorithm were chosen according to the recommendations of Angelis *et al.* (2001).

Simulations and Theorem 2.1 indicate that the design **L** is D-optimal when $n > 2p-5$ and $\rho \in [0,1)$, and sometimes when $n = 2p-5$ and $\rho < \alpha < 0.06$ for some α (in these situations the SA algorithm did not find D-better design than the design **L**). In the other cases, using the SA algorithm, we found D-better designs than the design **L**. We can observe that the inner product of any two columns of those designs is equal to ± 1 (for the vast majority of columns) or ± 3, and the same observation holds for the sum of elements in any column. Some examples of the best designs found by SA algorithm are given in the Supplementary materials (Appendix A). As an example, Figure 1 depicts the results of our simulations when $n = 15$, $\rho = 0.99$ and $p = 2, ..., 14$. For the other values of parameter ρ, the situation is similar as for $\rho = 0.99$. However, when there are D-better designs than the design **L**, SA algorithm finds sometimes different designs for different values of ρ.

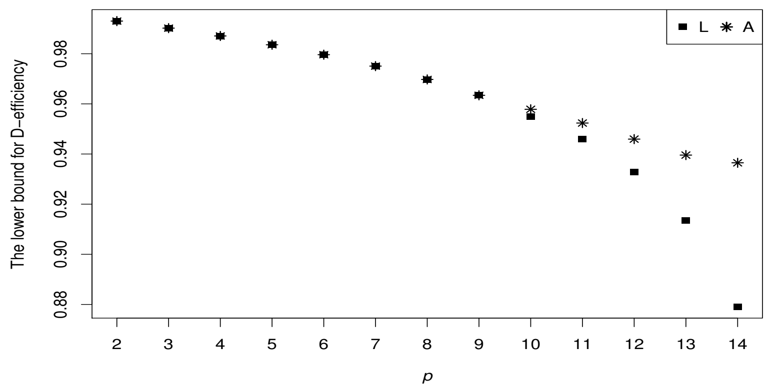

Figure 1: The lower bound for D-efficiency of design **L** (L) and the best designs found by SA algorithm (A) for $n = 15$ and $\rho = 0.99$.

For example, when $n = 15$ and $p = 10$, SA algorithm found, as the best design under D-optimality criterion, the design **T** for small values of $\rho > 0$, and the design **S** for the other values of this parameter (see Figure 2). The designs **T** and **S** are given in Appendix B.

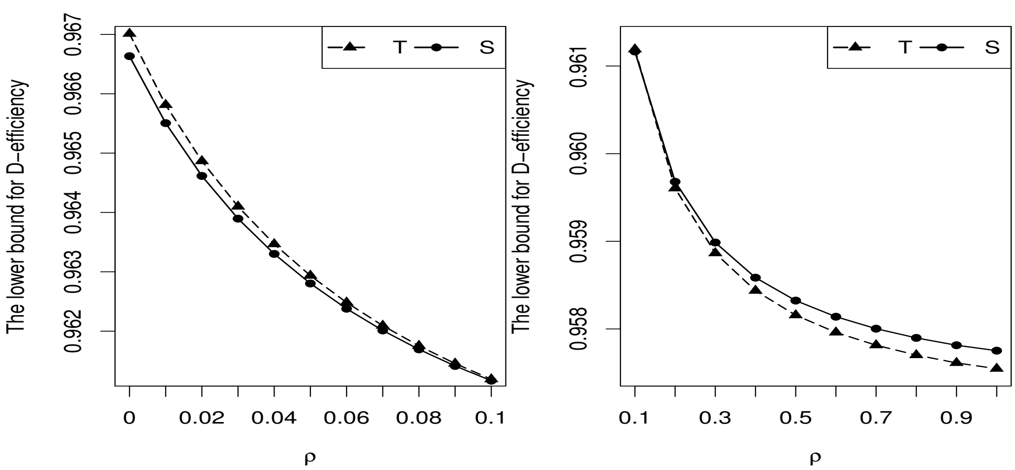

Figure 2: The lower bound for D-efficiency of the best designs **T** (T) and **S** (S) found by SA algorithm for $n = 15$ and $p = 10$.

These designs are D-better than the design $\mathbf{L}$ for "almost all" $\rho > 0$. It is important that the design $\mathbf{T}$, which seems to be D-optimal for certain small $\rho > 0$, is D-optimal, when $\rho = 0$ (it follows from Theorem in Galil and Kiefer, 1980), and the design $\mathbf{S}$, which seems to be D-optimal for the other values of ρ, is not D-optimal design for $\rho = 0$. This indicates that the D-optimal design for greater values of ρ does not have to be D-optimal when $\rho = 0$, and conversely, in some cases. The veracity of that conjecture is confirmed in the following section.

4. CASE STUDY

In this section we consider a special case where different designs are D-optimal for different values of parameter ρ. This (theoretically) confirms the conjecture from Section 3.

When $n = 7$ and $p = 6$, the simulations suggest that the design $\mathbf{L}$ is D-optimal for $\rho \in [0, 1/18]$, and the design ($-$ denotes -1 and $+$ represents 1)

$$\mathbf{A} = \begin{pmatrix} - & + & + & + & + & + \\ - & - & + & - & - & + \\ - & - & - & + & + & - \\ - & + & - & + & - & + \\ + & + & - & - & + & - \\ + & - & - & + & + & + \\ + & + & + & + & - & - \end{pmatrix} \tag{4.1}$$

is D-optimal for $\rho \in [1/18, 1)$. This information helped to prove the following theorem.

Theorem 4.1. *If* $\mathrm{Cov}(\mathbf{e}) = \sigma^2 \mathbf{G}$, *where* $\mathbf{G}$ *is given by* (1.1), *then any D-optimal design in* $\mathcal{M}_{7\times 6}(\{-1, 1\})$ *for* $\rho = 0$ *is not D-optimal design for* $\rho > 1/18$, *and conversely.*

Proof: Let $\mathbf{X}$ be an arbitrary D-optimal design for $\rho = 0$ in $\mathcal{M}_{7\times 6}(\{-1, 1\})$. The normalization (see Galil and Kiefer, 1980) refers to the following operations on $\mathbf{X}$: multiplying on the right by a diagonal matrix of ± 1's and/or a permutation matrix, which permutes rows and corresponding columns of $\mathbf{X}'\mathbf{X}$ and multiplies some entries of $\mathbf{X}'\mathbf{X}$ by -1. The results of Ehlich (1964) and Theorem in Galil and Kiefer (1980) imply the matrix $\mathbf{X}'\mathbf{X}$ is equal to $8\mathbf{I}_6 - \mathbf{1}_6\mathbf{1}_6'$ or to

$$\begin{pmatrix} 8\mathbf{I}_4 - \mathbf{1}_4\mathbf{1}_4' & -\mathbf{1}_4 & -\mathbf{1}_4 \\ -\mathbf{1}_4' & 7 & 3 \\ -\mathbf{1}_4' & 3 & 7 \end{pmatrix}$$

after normalization. We see that the normalization leaves $\det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$ unchanged, so we can assume that $\mathbf{X}'\mathbf{X}$ has one of the above forms. By Masaro and Wong (2008a), denote by $\mathcal{D}_4(7,6)$ the subclass of such designs. Proposition 5 (a) of Masaro and Wong (2008a) implies the design in that subclass, for which the sum of elements in each column is equal to -1, is D-optimal in $\mathcal{D}_4(7,6)$ for all $\rho > 0$. In the paragraph before Theorem 2.1, we noticed $\mathbf{L}'\mathbf{L} = 8\mathbf{I}_6 - \mathbf{1}_6\mathbf{1}_6'$ and $\mathbf{L}'\mathbf{1}_7 = -\mathbf{1}_6$. So, $\mathbf{L}$ is D-optimal in $\mathcal{D}_4(7,6)$ for all $\rho > 0$. Consider the design $\mathbf{A}$ given by (4.1). It can be calculated that $\mathbf{A}$ does not belong to $\mathcal{D}_4(7,6)$,

$$\det(\mathbf{A}'\mathbf{G}^{-1}\mathbf{A}) = c^6(61440 - 98304\,r)$$

and

$$\det(\mathbf{L}'\mathbf{G}^{-1}\mathbf{L}) = c^6(65536 - 196608\,r)\;,$$

where $c = 1/(1-\rho)$ and $r = \rho/(1+6\rho)$. Comparing these two determinants, we obtain $\mathbf{A}$ is D-better than $\mathbf{L}$ for all $\rho > 1/18$. Therefore, for all $\rho > 1/18$, the design $\mathbf{A}$ is D-better than any D-optimal design for $\rho = 0$ in $\mathcal{M}_{7\times 6}(\{-1,1\})$. So, the first part of the claim is proved. Let now $\mathbf{Y} \in \mathcal{M}_{7\times 6}(\{-1,1\})$ be an arbitrary D-optimal design for $\rho > 1/18$. From the above considerations, we conclude that for all $\rho > 1/18$,

$$\det(\mathbf{Y}'\mathbf{G}^{-1}\mathbf{Y}) \geqslant \det(\mathbf{A}'\mathbf{G}^{-1}\mathbf{A}) > \det(\mathbf{X}'\mathbf{G}^{-1}\mathbf{X})$$

for any D-optimal design $\mathbf{X}$ for $\rho = 0$. Thus, $\mathbf{Y}$ is not D-optimal, when $\rho = 0$. The proof is complete. □

Theorem 4.1 shows that we can not assume a priori that there is a design which is optimal for all $\rho \in [0,1)$. This indicates the reasonableness of searching optimal designs for different values of parameter ρ.

5. CONCLUSION

In this paper we showed that the design $\mathbf{L}$ constructed by Masaro and Wong (2008a) is highly D-efficient in many cases when the number of observations $n \equiv 3 \pmod 4$. Simulations conducted by SA algorithm (Angelis *et al.*, 2001) suggest that the design $\mathbf{L}$ is D-optimal when the number of observations is appropriately large or appropriately larger than the number of objects. In the other cases, however, we found D-better designs than $\mathbf{L}$. Nevertheless, the "D-efficiency" advantage of those designs over $\mathbf{L}$ is negligible for appropriately large n. For smaller number of n (e.g., $n = 7, 11, 15$), this advantage is evident, and hence the best designs found by SA algorithm are listed in the Supplementary materials. Even though those designs or the design $\mathbf{L}$ are not D-optimal, they may be safety used in practice through their high D-efficiency.

APPENDIX A. SUPPLEMENTARY MATERIAL

Supplementary material lists the examples of the best chemical balance weighing designs under D-optimality criterion found by simulated annealing algorithm. It is available at the webpage `http://www.staff.amu.edu.pl/~ls/str_en.html`.

APPENDIX B. DESIGNS T AND S

Let $-$ denote -1 and $+$ represent 1.

$$\mathbf{T} = \begin{pmatrix}
- & + & + & + & + & + & + & + & + & + \\
- & - & + & - & + & - & - & + & - & + \\
+ & - & - & + & - & - & + & + & - & - \\
- & - & + & - & + & - & + & - & + & - \\
- & - & - & - & - & + & - & + & + & - \\
- & - & - & + & - & - & + & - & + & + \\
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- & + & + & - & - & - & + & + & - & - \\
+ & + & - & - & + & + & + & + & + & - \\
+ & + & + & + & - & - & - & + & + & + \\
- & + & + & + & - & + & - & - & - & -
\end{pmatrix}, \qquad
\mathbf{S} = \begin{pmatrix}
- & - & - & - & + & + & - & + & - & - \\
- & + & - & + & + & + & - & + & + & + \\
+ & + & - & + & - & + & - & - & - & - \\
+ & + & - & - & - & - & + & + & - & - \\
+ & - & - & + & + & + & + & + & - & + \\
- & - & - & - & - & + & + & - & + & - \\
+ & + & + & - & + & + & + & - & - & + \\
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+ & - & - & - & + & - & - & - & + & + \\
- & - & + & + & + & - & + & - & - & - \\
- & - & + & + & - & - & - & + & - & + \\
+ & + & + & - & + & - & - & + & + & - \\
+ & - & + & + & - & + & - & - & + & -
\end{pmatrix}.$$

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