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Some refinements on Fedorov's algorithms for constructing D-optimal designs

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Abstract. Well-known and widely used algorithms for constructing D-optimal designs are Fedorov's sequential algorithm and Fedorov's exchange algorithm. In this paper, we modify these two algorithms by adding or exchanging two or more points simultaneously at each step. This will significantly reduce the number of steps needed to construct a D-optimal design. We also prove the convergence of the proposed sequential algorithm to a D-optimal design. Optimal designs for rational regression are used as an illustration.

1 Introduction

The modern theory of optimal design started with the pioneering works of Kiefer (1959, 1961a, 1961b, 1962, 1971 and 1974) and Kiefer and Wolfowitz (1959, 1960) who made a number of important contributions to the theory. Their main result is the general equivalence theorem, which plays a central role in constructing D-optimal designs.

There are two well-known approaches for constructing D-optimal designs. The first approach starts from an initial n-point design (an arbitrary design with a nonsingular information matrix). Then new points are added to the design following a certain rule. These algorithms are known as *sequential algorithms*. Generally, the number of design points for such algorithms is increasing. Fedorov (1972) appears to have been the first to develop a general algorithm for obtaining D-optimal designs. He gave a sequence of continuous designs which converges monotonically to a D-optimal design. Wynn (1970) provided another algorithm for constructing a converging sequence of discrete (exact) designs. He also obtained bounds which can be used to find out how close one is to an optimal design without knowing the true optimal design. Pazman (1974) gave a different proof for the Wynn's algorithm. Covey-Crump and Silvey (1970), Dykstra (1971), and Hebble and Mitchell (1971) suggested algorithms similar to Wynn's, but did not give convergence proofs. Tsay (1976) gave a general procedure for constructing D-optimal designs, which includes Wynn's algorithm as a special case. Silvey, Titterington

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and Torsney (1978) gave an additional algorithm, named the multiplicative algorithm. They also proved that this algorithm converges monotonically to a D-optimal design. Recently, Yu (2011) proposed a cocktail algorithm based on Fedorov's algorithm and the multiplicative algorithm. Pronzato (2003) and Herman and Pronzato (2007) proposed some inequalities in order to remove non-optimal support points.

The second procedure for constructing D-optimal designs starts with a nonsingular n-point design. Next, it adds and deletes one or more observations points following a certain rule. These algorithms are called *exchange algorithms*. The number of design points for such algorithms remains constant. Unfortunately, to this day there is no proof that guarantees the convergence of such algorithms to a D-optimal design. However, there is a strong numerical evidence that they converge to a D-optimal design very fast (sometimes even in few steps). Historically, the first exchange algorithm for the construction of exact D-optimal design was developed by Fedorov (1972). The details of this algorithm is given in the Section 3 of this paper. Another exchange algorithm, due to Mitchell and Miller (1970), begins with an arbitrary n-point design. Then it finds a candidate point which maximizes the variance function and adds it to the design. Next, it looks for a point from the design points which minimizes the variance function and removes it form the design. Mitchell (1974) proposed the DETMAX algorithm which allows the value of n, the number of the design points, to increase and decrease in order to get a better search within the design region. However, constraints are placed on the amount of changes in the value of n, and the algorithm forces a return to an n-point design. Another exchange algorithm for constructing D-optimal designs is the k-exchange algorithm due to Johnson and Nachtsheim (1983). The foregoing authors figured out that the points selected for deletion by the Fedorov exchange algorithm are normally not the ones with the lowest variance of prediction. Instead of considering all candidate points, they suggested to use a set of k points with the lowest variance. Then each iteration is broken into k steps. Inside each of these k steps a couple is exchanged if the determinant of the information matrix of the new design is increased. The selection of the k-value is difficult and in most cases problem-dependent. Common values are $k = 3$ or $k = 4$ (Johnson and Nachtsheim, 1983). Meyer and Nachtsheim (1995) later advised to select k such that $k \leq n/4$. Setting $k = n$ gives Cook and Nachtsheim (1980) algorithm. An additional exchange algorithm is the kl-exchange developed by Atkinson and Donev (1989). This algorithm reduces the list of points to be added and deleted. The use of the k points with the lowest variance of prediction is similar to the k-exchange procedure. In addition to this, it only considers the l candidates with the highest variance of prediction among the support points. The main advantage of the k-exchange algorithm and the kl-exchange algorithm is that they speed up in an effective way Fedorov's exchange algorithm. However, the quality of design is not always as good as the one obtained from Fedorov's original exchange algorithm (Cook and Nachtshem, 1980; Johnson and Nachtsheim, 1983; Atkinson and Donev, 1989; Triefenbach, 2008). Nguyen and Miller (1992) showed that, the worse the starting design, the longer it takes for this algorithm to converge to the D-optimal design. Meyer and Nachtsheim (1995) described a cyclic coordinate-exchange algorithm, a generalization k-exchange algorithm. We refer the reader to the ordinal papers for more details and comparisons between existing algorithms.

The aforementioned algorithms for constructing D-optimal designs are single point algorithms. That is, at each step only one point can be added or exchanged simultaneously. However, in many practical situations it may be possible to add or exchange two or more points simultaneously. Typically, such cases happen when there is a certain symmetry in the design (Atwood, 1973; Al Labadi and Zhen, 2010). It must be noted, however, that most the examples available in the literature are symmetric designs. See, for example, among others, Fedrov (1972, Chapters 2 and 3), Wynn (1970), Liski, Mandal, Shah and Sinha (2002, p. 3), and Harman and Pronzato (2007).

The main objective of this paper is to extend Fedorov's sequential algorithm and Fedorov's exchange algorithms in order to add or exchange two or more points simultaneously at each step. Achieving this goal reduces the computational time required to construct a D-optimal design via Fedorov's algorithms. For simplicity, we will consider the case when two points are added or exchanged simultaneously at each step. The general case follows similarly.

The remainder of the paper is organized as follows. In Section 2, we introduce some preliminary material about optimal design theory. In Section 3, Fedorov's original algorithms for constructing D-optimal designs are reviewed. The steps of the modified Fedorov's sequential and exchange algorithms are presented in Section 4 and Section 5, respectively. Our main theoretical results come in the following two sections. First, some matrix algebra and optimal design theory results are developed in Section 6. We then prove the convergence modified Fedorov's sequential algorithm to a D-optimal design in Section 7. An example illustrating and comparing the modified algorithms is presented in Section 8. Finally, some concluding remarks are made in Section 9.

2 Optimal design theory

In this section, we introduce necessary concepts and classical theory of D-optimal design. Following the setup of Kiefer and Wolfowitz (1959), let $f_1, f_2, \ldots, f_p$ be p linearly independent continuous functions on a compact region $\mathscr{X}$. We assume that at each point x in $\mathscr{X}$ a random variable $\mathbf{Y}_x$ (response) is defined such that

$$\mathbf{E}(\mathbf{Y}_x) = \boldsymbol{\beta}'\mathbf{f}(x) = \sum_{i=1}^{p} \beta_i f_i(x),$$

where $\mathbf{f}(x)$ is a $p \times 1$ column vector of the functions f_i $(i = 1, \ldots, p)$ evaluated at x and $\boldsymbol{\beta}$ is a $p \times 1$ column vector of unknown parameters β_i $(i = 1, \ldots, p)$. We assume also that $\mathrm{Var}(\mathbf{Y}_x) = \sigma^2$, $\mathrm{Cov}(\mathbf{Y}_{x_1}, \mathbf{Y}_{x_2}) = 0$ for x, x_1, x_2 in $\mathscr{X}$ ($x_1 \neq x_2$). If observations $\{\mathbf{Y}_{x_i}\}_{i=1}^{N}$ are taken, then we have the corresponding $N \times p$ design matrix $\mathbf{X}$ whose ith row is the vector $\mathbf{f}'(x_i)$. If the unknown parameter vector β is estimated by the method of *least squares*, then the resulting estimator $\hat{\beta}$ is known to be the best linear unbiased estimator and its covariance matrix is $\sigma^2(\mathbf{X}'\mathbf{X})^{-1}$, assuming that the matrix $\mathbf{X}'\mathbf{X}$ is non-singular. The variance of the best linear unbiased estimator of $\boldsymbol{\beta}'\mathbf{f}(x)$ is thus equal to

$$\sigma^2 \mathbf{f}'(x)\left(\mathbf{X}'\mathbf{X}\right)^{-1}\mathbf{f}(x). \tag{2.1}$$

We always distribute the N observations in (approximately) equal portions among $n \geq p$ design points. A design ξ can be written as

$$\xi = \begin{Bmatrix} x_1, & x_2, & \dots, & x_n \\ w_1, & w_2, & \dots, & w_n \end{Bmatrix},$$

where the n support points $x_1, x_2, \dots, x_n$ are elements of the design region $\mathscr{X}$ and the associated weights $w_1, w_2, \dots, w_n$ are nonnegative real numbers which sum to one. If all the associated weights are rational numbers (i.e., multiples of $1/n$), then the resulting design is called a *discrete* (i.e., exact) design. Removing this restriction, we can extend this idea to a design measure (Kiefer and Wolfowitz, 1959; John and Draper, 1975) which satisfies, in general: $\xi(A) \geq 0$, $A \subset \mathscr{X}$, and $\int_{\mathscr{X}} \xi(dx) = 1$. The resulting design is called a *continuous* (i.e., approximate) design.

A design ξ is *symmetric* if, for some natural number k, it has either of the following forms:

1. $\xi = \begin{Bmatrix} x_1, & x_2, & \dots, & x_k, & -x_k, & \dots, & -x_2, & -x_1 \\ w_1, & w_2, & \dots, & w_k, & w_{k+1}, & \dots, & w_{n-1}, & w_n \end{Bmatrix}$ when $n = 2k$,

or

2. $\xi = \begin{Bmatrix} x_1, & x_2, & \dots, & x_k, & 0, & -x_k, & \dots, & -x_2, & -x_1 \\ w_1, & w_2, & \dots, & w_k, & w_{k+1}, & w_{k+2}, & \dots, & w_{n-1}, & w_n \end{Bmatrix}$ when $n = 2k + 1$.

For an arbitrary design ξ, the information matrix is defined as

$$\mathbf{M}(\xi) = \int_{\mathscr{X}} \mathbf{f}(x)\mathbf{f}'(x)\xi(dx).$$

Throughout this paper, an n-point design will be denoted by ξ_n. The subscript denotes the number of points in the design. For any discrete design ξ_n we will attach a mass of $1/n$ to each point in the design. The design matrix $\mathbf{X}$ corresponding to a design ξ_n will be given the same subscript. If ξ_n is a discrete (exact) design, then the information matrix for this n-point design satisfies the following equation

$$n\mathbf{M}(\xi_n) = \mathbf{X}_n'\mathbf{X}_n.$$

For a general design ξ, define

$$d(x, \xi) = \mathbf{f}'(x)\mathbf{M}^{-1}(\xi)\mathbf{f}(x).$$

Thus,

$$d(x, \xi_n) = n\mathbf{f}'(x)\big(\mathbf{X}_n'\mathbf{X}_n\big)^{-1}\mathbf{f}(x).$$

It can be seen that the variance of the best linear unbiased estimator of $\boldsymbol{\beta}'\mathbf{f}(x)$ in (2.1) is now equal to $(\sigma^2/n)d(x, \xi_n)$.

A design ξ^* is D-optimal if and only if $\mathbf{M}(\xi^*)$ is non-singular and $\det\{\mathbf{M}(\xi^*)\} = \max_\xi \det\{\mathbf{M}(\xi)\}$. ξ^* is G-optimal if and only if $\max_{x\in\mathscr{X}} d(x, \xi^*) = \min_\xi \max_{x\in\mathscr{X}} d(x, \xi)$. Kiefer and Wolfowitz (1959) proved the following *general equivalence theorem*.

Theorem 2.1. *The following three conditions are equivalent*: (i) ξ^* *is D-optimal*, (ii) ξ^* *is G-optimal*, (iii) $\max_{x\in\mathscr{X}} d(x, \xi^*) = p$.

The major use of this Theorem 2.1 is to provide a simple way for constructing D-optimal designs. Simply, if condition (iii) is satisfied, then the design is D-optimal.

3 Fedorov's original algorithms

In this section, we discuss Fedorov's original sequential and exchange algorithms for constructing D-optimal designs.

3.1 Fedorov's original sequential algorithm

In order to improve the current design ξ_n, Fedorov (1972, Chapter 2) suggested adding to the design sequentially that point of the design region $\mathscr{X}$ where the variance function $d(x, \xi_n)$ achieves its maximum. The steps of Fedorov's original sequential algorithm are:

1. Find an initial non-degenerate n_0-point design ξ_{n_0} on $\mathscr{X}$, and $i = n_0$.
2. Compute $\mathbf{M}(\xi_i)$, $\mathbf{M}^{-1}(\xi_i)$ and $d(x, \xi_i)$.
3. Find x_{i+1} such that

$$d(x_{i+1}, \xi_i) = \max_x d(x, \xi_i) = \bar{d}(\xi_i).$$

   If $\bar{d}(\xi_i)$ is sufficiently close to p, stop: the design ξ_{i+1} is almost D-optimal, where the design ξ_{i+1} is defined as in step 5.
4. Otherwise, let

$$\alpha_i = \frac{\bar{d}(\xi_i) - p}{p(\bar{d}(\xi_i) - 1)}.$$

5. Define a new design by $\xi_{i+1} = (1 - \alpha_i)\xi_i + \alpha_i\xi(x_i)$, where $\xi(x_{i+1})$ is a design consisting of one point x_{i+1}.
6. Set $i = i + 1$ and return to step 2.

It is worth mentioning that the value of α_i in step 4 of the algorithm is the best value that maximizes the determinant of the information matrix of the new design. The selection of α in this way makes the determinant of the information matrix keep increasing. Note that, the choice $\alpha_i = 1/n$ corresponds to Wynn's algorithm (1970).

3.2 Fedorov's original exchange algorithm

Fedorov (1972, Chapter 3) proposed an exchange algorithm for constructing D-optimal designs. This algorithm starts with an arbitrary non-degenerate n-point design ξ_n^0. During the jth iteration (exchange) a point, say x_i, is deleted from the design and another point $x \in \chi$ is added in a way which leads to a maximal increase of $\det(\mathbf{X}_n'\mathbf{X}_n)$. Thus the number of design points remains constant.

As mentioned earlier, in both Fedorov's algorithms only one point is added or exchanged at each step. However, in many practical situations the maximum of the variance function $d(x, \xi_n)$ may be achieved at two different points. This case typically happens when there is a symmetry in the variance function (or equivalently a symmetry in the response function **f**). In this case, adding/exchanging two points simultaneously may reduce the number of iterations (exchanges) needed to construct D-optimal designs by a half.

4 Modified Fedorov's sequential algorithm

In the section, we describe the modified Fedorov's sequential algorithm. The proof that this algorithm generates a D-optimal designs is given in Section 7. The steps of the modified Fedorov's sequential algorithm are:

1. Find an initial non-degenerate symmetric n_0-point design ξ_{n_0} on $\mathscr{X}$, and $i = n_0$.
2. Compute $\mathbf{M}(\xi_i)$, $\mathbf{M}^{-1}(\xi_i)$ and $d(x, \xi_i)$.
3. Find x_{i+1} and x_{i+2} such that
$$d(x_{i+1}, \xi_i) = d(x_{i+2}, \xi_i) = \max_x d(x, \xi_i) = \bar{d}(\xi_i).$$
If $\bar{d}(\xi_i)$ is sufficiently close to p, stop: the design ξ_{i+2} is almost D-optimal, where the design ξ_{i+2} is defined as in step 5. Note, by symmetry, $x_{i+2} = -x_{i+1}$.
4. Otherwise, choose α_i that maximizes $\det\{\mathbf{M}(\xi_{i+2})\}$. This can be done either numerically or by using an approximate value
$$\alpha_i = \big(\bar{d}(\xi_i) - p\big)/\big(2p\big(\bar{d}(\xi_i) - 1\big)\big).$$
(The approximate value of α_i is derived in Section 6 of the present paper.)
5. Define a new design by $\xi_{i+2} = (1 - 2\alpha_i)\xi_i + \alpha_i\xi(x_{i+1}) + \alpha_i\xi(x_{i+2})$, where $\xi(x_{i+1})$ and $\xi(x_{i+2})$ are one-point designs.
6. Set $i = i + 2$ and return to step 2.

5 Modified Fedorov's exchange algorithm

The basic idea of the modified Fedorov's exchange algorithm for constructing D-optimal symmetric designs is to select a pair of points, say $\pm x_i$, from the design ξ_n^j and replace it with another pair of points, say $\pm x$, from the design region χ which leads to a maximal increase of $\det(\mathbf{X}_n'\mathbf{X}_n)$. To formulate this into a mathematical equation, let the matrix $(\mathbf{X}_n'\mathbf{X}_n)^j$ be the matrix that corresponds to the design ξ_n^j. Then the new matrix $(\mathbf{X}_n'\mathbf{X}_n)^{j+1}$ can be obtained by the equation:

$$\begin{aligned}(\mathbf{X}_n'\mathbf{X}_n)^{j+1} = (\mathbf{X}_n'\mathbf{X}_n)^j &- f(x_i)f'(x_i) - f(-x_i)f'(-x_i) \\ &+ f(x)f'(x) + f(-x)f'(-x).\end{aligned} \tag{5.1}$$

The pair of points $\pm x \in \chi$ is selected so that the determinant of the matrix $(\mathbf{X}_n'\mathbf{X}_n)^{j+1}$ in (5.1) is maximal. This determinant can be viewed as a function in x.

Now we describe the main steps for numerical implementation of the modified Fedorov's exchange algorithm. The required steps are:

1. Start with a randomly non-degenerate symmetric n-point design ξ_n^0.
2. Set $j = 0$ and compute $(\mathbf{X}_n'\mathbf{X}_n)^j$ and $\det\{(\mathbf{X}_n'\mathbf{X}_n)^j\}$.
3. Compute $\max_{x\in\chi} \det\{(\mathbf{X}_n'\mathbf{X}_n)^{j+1}\}$ for all pairs $\pm x_i$ in the design, where $(\mathbf{X}_n'\mathbf{X}_n)^{j+1}$ is given by (5.1). Choose the pairs $\pm x_i$ and $\pm x$ which achieve
$$\max_{x_i\in\xi_n^j}\max_{x\in\chi}\det\{(\mathbf{X}_n'\mathbf{X}_n)^{j+1}\},$$
and replace $\pm x_i$ by $\pm x$.
4. After each exchange, a new design ξ_n^{j+1} is obtained. We also recompute $(\mathbf{X}_n'\mathbf{X}_n)^{j+1}$ and $\det\{(\mathbf{X}_n'\mathbf{X}_n)^{j+1}\}$.
5. Set $j = j + 1$ and repeat steps 3–4 until the largest value of
$$\Delta = \frac{\det\{(\mathbf{X}_n'\mathbf{X}_n)^{j+1}\} - \det\{(\mathbf{X}_n'\mathbf{X}_n)^j\}}{\det\{(\mathbf{X}_n'\mathbf{X}_n)^j\}}$$
is sufficiently close to zero.

6 Preliminary lemmas

This section contains some fundamental lemmas that will be used to prove the convergence of the modified algorithm to a D-optimal design.

Lemma 6.1. *Let* $\mathbf{W}$ *be a non-singular* $p \times p$ *matrix and* $\mathbf{V}$ *be a* $p \times q$ *matrix. Then for any real number* λ

$$\det\{\mathbf{W} + \lambda\mathbf{V}\mathbf{V}'\} = \det\{\mathbf{W}\}\det\{\mathbf{I}_q + \lambda\mathbf{V}'\mathbf{W}^{-1}\mathbf{V}\}.$$

The proof can be found in Fedorov (1972), page 100.

Corollary 1. *If* $\mathbf{W}$ *is a* $p \times p$ *symmetric positive definite matrix and* $\mathbf{a}$, $\mathbf{b}$ *are two* $p \times 1$ *column vectors, then for any real number* λ

$$\det\{\mathbf{W} + \lambda \mathbf{a}\mathbf{a}' + \lambda \mathbf{b}\mathbf{b}'\} = \big[1 + \lambda \mathbf{a}'\mathbf{W}^{-1}\mathbf{a} + \lambda \mathbf{b}'\mathbf{W}^{-1}\mathbf{b} + \lambda^2 \mathbf{a}'\mathbf{W}^{-1}\mathbf{a}\mathbf{b}'\mathbf{W}^{-1}\mathbf{b} - \lambda^2 \big(\mathbf{a}'\mathbf{W}^{-1}\mathbf{b}\big)^2\big] \det\{\mathbf{W}\}. \tag{6.1}$$

Proof. The proof follows by setting $\mathbf{V} = (\mathbf{a}\ \mathbf{b})$ in Lemma 6.1. □

Lemma 6.2. *Let* $\mathbf{M}(\xi_n)$ *be the information matrix of a non-degenerate design* ξ_n. *Let* $\mathbf{M}(\xi(x_{n+1}))$ *and* $\mathbf{M}(\xi(x_{n+2}))$ *be the information matrices of the one-point designs* $\xi(x_{n+1})$ *and* $\xi(x_{n+2})$, *respectively. Then*

$$\begin{aligned}\det\{\mathbf{M}(\xi_{n+2})\} &= (1-2\alpha)^p \Bigg[1 + \left(\frac{2\alpha}{1-2\alpha}\right)\bar{d}(\xi_n) + \left(\frac{\alpha}{1-2\alpha}\right)^2 \bar{d}^2(\xi_n) \\ &\quad - \left(\frac{\alpha}{1-2\alpha}\right)^2 \big(\mathbf{f}'(x_{n+1})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+2})\big)^2\Bigg] \det\{\mathbf{M}(\xi_n)\},\end{aligned}$$

where $\xi_{n+2} = (1-2\alpha)\xi_n + \alpha\xi(x_{n+1}) + \alpha\xi(x_{n+2})$ *and* $\bar{d}(\xi_n) = \max_x d(x, \xi_n) = d(x_{n+1}, \xi_n) = d(x_{n+2}, \xi_n)$.

Proof. From the definition of information matrix, we have

$$\begin{aligned}\mathbf{M}(\xi_{n+2}) &= (1-2\alpha)\mathbf{M}(\xi_n) + \alpha\mathbf{M}\big(\xi(x_{n+1})\big) + \alpha\mathbf{M}\big(\xi(x_{n+2})\big) \\ &= (1-2\alpha)\Bigg[\mathbf{M}(\xi_n) + \frac{\alpha}{1-2\alpha}\mathbf{f}(x_{n+1})\mathbf{f}'(x_{n+1}) \\ &\quad + \frac{\alpha}{1-2\alpha}\mathbf{f}(x_{n+2})\mathbf{f}'(x_{n+2})\Bigg].\end{aligned}$$

Therefore,

$$\begin{aligned}\det\{\mathbf{M}(\xi_{n+2})\} = (1-2\alpha)^p \det\Bigg\{&\mathbf{M}(\xi_n) + \frac{\alpha}{1-2\alpha}\mathbf{f}(x_{n+1})\mathbf{f}'(x_{n+1}) \\ &+ \frac{\alpha}{1-2\alpha}\mathbf{f}(x_{n+2})\mathbf{f}'(x_{n+2})\Bigg\}.\end{aligned}$$

Setting $\mathbf{W} = \mathbf{M}(\xi_n)$, $\mathbf{a} = \mathbf{f}(x_{n+1})$, $\mathbf{b} = \mathbf{f}(x_{n+2})$ and $\lambda = \alpha/(1-2\alpha)$ in (6.1), we obtain

$$\begin{aligned}\det\{\mathbf{M}(\xi_{n+2})\} \\ = (1-2\alpha)^p\end{aligned}$$

$$
\begin{aligned}
&\times \Big[1 + \frac{\alpha}{1-\alpha}\mathbf{f}'(x_{n+1})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+1}) \\
&\quad + \frac{\alpha}{1-2\alpha}\mathbf{f}'(x_{n+2})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+2}) \\
&\quad + \left(\frac{\alpha}{1-2\alpha}\right)^2 \mathbf{f}'(x_{n+1})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+1})\mathbf{f}'(x_{n+2})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+2}) \\
&\quad - \left(\frac{\alpha}{1-2\alpha}\right)^2 \left(\mathbf{f}'(x_{n+1})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+2})\right)^2\Big] \det\{\mathbf{M}(\xi_n)\} \\
&= (1-2\alpha)^p\Big[1 + \frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n) + \left(\frac{\alpha}{1-2\alpha}\right)^2 \bar{d}^2(\xi_n) \\
&\quad - \left(\frac{\alpha}{1-2\alpha}\right)^2 \left(\mathbf{f}'(x_{n+1})\mathbf{M}^{-1}(\xi_n)\mathbf{f}(x_{n+2})\right)^2\Big] \det\{\mathbf{M}(\xi_n)\}. \qquad \square
\end{aligned}
$$

Corollary 2.

$$
\det\{\mathbf{M}(\xi_{n+2})\} \geq (1-2\alpha)^p\left[1 + \frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right]\det\{\mathbf{M}(\xi_n)\}. \tag{6.2}
$$

In the next lemma we show that it is always possible to find an α for which $\det\{\mathbf{M}(\xi_{n+2})\} > \det\{\mathbf{M}(\xi_n)\}$, if the design ξ_n is not D-optimal.

Lemma 6.3. *For a given design ξ_n which is not D-optimal, we have*

$$
\begin{aligned}
\det\{\mathbf{M}(\xi_{n+2})\} &\geq \max_\alpha\left[(1-2\alpha)^p\left(1 + \frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right)\det\{\mathbf{M}(\xi_n)\}\right] \\
&= \left[\frac{\bar{d}(\xi_n)}{p}\right]^p \times \left[\frac{p-1}{\bar{d}(\xi_n)-1}\right]^{p-1} \det\{\mathbf{M}(\xi_n)\} \\
&> \det\{\mathbf{M}(\xi_n)\},
\end{aligned}
$$

where $\xi_{n+2} = (1-2\alpha)\xi_n + \alpha\xi(x_{n+1}) + \alpha\xi(x_{n+2})$ and $\bar{d}(\xi_n) = \max_x d(x,\xi_n) = d(x_{n+1},\xi_n) = d(x_{n+2},\xi_n)$.

Proof. Denote

$$
F = (1-2\alpha)^p\left(1 + \frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right)\det\{\mathbf{M}(\xi_n)\},
$$

then from Corollary 2 we have

$$
\begin{aligned}
\det\{\mathbf{M}(\xi_{n+2})\} \;&\geq\; \max_\alpha\left[(1-2\alpha)^p\left(1 + \frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right)\det\{\mathbf{M}(\xi_n)\}\right] \\
&:= \max_\alpha F.
\end{aligned} \tag{6.3}
$$

To find the α which maximizes F, note that

$$
\begin{aligned}
\frac{\partial}{\partial\alpha}\log F &= \frac{\partial}{\partial\alpha}\log\left\{(1-2\alpha)^p\left(1+\frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right)\det\{\mathbf{M}(\xi_n)\}\right\}\\
&= \frac{\partial}{\partial\alpha}\left\{p\log(1-2\alpha)+\log\left(1+\frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right)+\log\det\{\mathbf{M}(\xi_n)\}\right\}\\
&= \frac{\partial}{\partial\alpha}\{p\log(1-2\alpha)+\log(1-2\alpha+2\alpha\bar{d}(\xi_n))-\log(1-2\alpha)\\
&\qquad +\log\det\{\mathbf{M}(\xi_n)\}\}\\
&= \frac{2\bar{d}(\xi_n)-2}{1-2\alpha+2\alpha\bar{d}(\xi_n)}-\frac{2p-2}{1-2\alpha}.
\end{aligned}
\tag{6.4}
$$

Equating the right-hand side of (6.4) to 0, yields the solution for the α.

$$
\frac{2\bar{d}(\xi_n)-2}{1-2\alpha+2\alpha\bar{d}(\xi_n)}=\frac{2p-2}{1-2\alpha}\quad\Rightarrow\quad \alpha_n=\frac{\bar{d}(\xi_n)-p}{2p[\bar{d}(\xi_n)-1]}.
\tag{6.5}
$$

Since by assumption the design ξ_n is not D-optimal, we have $\bar{d}(\xi_n)-p>0$. It follows that $\alpha_n>0$.

On the other hand,

$$
\begin{aligned}
\frac{\partial^2}{\partial\alpha^2}\log(F)\Big|_{\alpha=\alpha_n} &= \frac{\partial}{\partial\alpha}\left\{\frac{2(\bar{d}(\xi_n)-1)}{1-2\alpha+2\alpha\bar{d}(\xi_n)}-\frac{2(p-1)}{1-2\alpha}\right\}\Big|_{\alpha=\alpha_n}\\
&= -\frac{4(\bar{d}(\xi_n)-1)^2}{(1-\alpha+\alpha\bar{d}(\xi_n))^2}-\frac{4(p-1)}{(1-\alpha)^2}\Big|_{\alpha=\alpha_n}\\
&< 0.
\end{aligned}
$$

Therefore, α_n corresponds to the maximum of $\log F$. Thus,

$$
\begin{aligned}
\max_{\alpha}\log F &= \max_{\alpha}\log\left\{(1-2\alpha)^p\left(1+\frac{2\alpha}{1-2\alpha}\bar{d}(\xi_n)\right)\det\{\mathbf{M}(\xi_n)\}\right\}\\
&> \log\det\{\mathbf{M}(\xi_n)\}.
\end{aligned}
\tag{6.6}
$$

Setting α_n defined by (6.5) into (6.2) we obtain, after a simple calculation,

$$
\begin{aligned}
F|_{\alpha=\alpha_n} &= \left(1-2\cdot\frac{\bar{d}(\xi_n)-p}{2[\bar{d}(\xi_n)-1]p}\right)^p\\
&\quad\times\left\{1+2\cdot\frac{\bar{d}(\xi_n)-p}{2[\bar{d}(\xi_n)-1]p}\Big/\left(1-2\cdot\frac{\bar{d}(\xi_n)-p}{2[\bar{d}(\xi_n)-1]p}\right)\bar{d}(\xi_n)\right\}\\
&\quad\times\det\{\mathbf{M}(\xi_n)\}\\
&= \left[\frac{\bar{d}(\xi_n)}{p}\right]^p\times\left[\frac{p-1}{\bar{d}(\xi_n)-1}\right]^{p-1}\det\{\mathbf{M}(\xi_n)\}.
\end{aligned}
\tag{6.7}
$$

Combining (6.3), (6.6) and (6.7) finishes the proof of the lemma. □

7 Convergence of modified Fedorovs's sequential algorithm

In this section, we show that the modified Fedorov's sequential algorithm converges to a D-optimal design.

Theorem 7.1. *For the sequence of designs constructed by the modified Fedorov's algorithm, we have*

$$\lim_{n\to\infty} \det\{M(\xi_n)\} = \det\{M(\xi^*)\},$$

where ξ^* is a D-optimal design.

Proof. Suppose the initial design ξ_{n_0} itself is not D-optimal. Then, by Lemma 6.3 and the definition of D-optimality,

$$\det\{\mathbf{M}(\xi_{n_0})\} < \det\{\mathbf{M}(\xi_{n_0+2})\} \leq \cdots \leq \det\{\mathbf{M}(\xi_n)\} \leq \cdots \leq \det\{\mathbf{M}(\xi^*)\}.$$

As is well known, any bounded monotone nondecreasing sequence converges. It follows that the sequence

$$\det\{\mathbf{M}(\xi_{n_0})\}, \det\{\mathbf{M}(\xi_{n_0+2})\}, \ldots, \det\{\mathbf{M}(\xi_n)\}, \ldots \tag{7.1}$$

converges to some limit $L \leq \det\{\mathbf{M}(\xi^*)\}$. Therefore, it is sufficient to show that

$$\det\{\mathbf{M}(\xi^*)\} = L.$$

Let us assume that

$$L < \det\{\mathbf{M}(\xi^*)\}. \tag{7.2}$$

This means that the designs $\xi_{n_0}, \xi_{n_0+2}, \ldots, \xi_n, \ldots$ all are not D-optimal, and

$$\det\{\mathbf{M}(\xi_{n_0})\} < \det\{\mathbf{M}(\xi_{n_0+2})\} < \cdots < \det\{\mathbf{M}(\xi_n)\} < \cdots < L.$$

In view of the convergence of the sequence (7.1), for any small positive number γ there is an n^* such that for any $n > n^*$ the following inequality holds:

$$0 < \det\{\mathbf{M}(\xi_{n+2})\} - \det\{\mathbf{M}(\xi_n)\} \leq \gamma. \tag{7.3}$$

By Lemma 6.3,

$$\begin{aligned}
&\det\{\mathbf{M}(\xi_{n+2})\} - \det\{\mathbf{M}(\xi_n)\} \\
&\quad \geq \left[\frac{\bar{d}(\xi_n)}{p}\right]^p \times \left[\frac{p-1}{\bar{d}(\xi_n)-1}\right]^{p-1} \det\{\mathbf{M}(\xi_n)\} - \det\{\mathbf{M}(\xi_n)\} > 0 \\
&\quad = \det\{\mathbf{M}(\xi_n)\}\left[\left[\frac{\bar{d}(\xi_n)}{p}\right]^p \times \left[\frac{p-1}{\bar{d}(\xi_n)-1}\right]^{p-1} - 1\right] \\
&\quad > 0.
\end{aligned} \tag{7.4}$$

Thus by (7.3) and (7.4), we have

$$0 < \det\{\mathbf{M}(\xi_n)\}\left[\left(\frac{\bar{d}(\xi_n)}{p}\right)^p \times \left(\frac{p-1}{\bar{d}(\xi_n)-1}\right)^{p-1} - 1\right] \leq \gamma,$$

or equivalently, setting $\delta_n = \bar{d}(\xi_n) - p$,

$$0 < \det\{\mathbf{M}(\xi_n)\}\left[\left(\frac{\delta_n + p}{p}\right)^p \left(\frac{p-1}{\delta_n + (p-1)}\right)^{p-1} - 1\right] \leq \gamma. \tag{7.5}$$

Inequality (7.5) can be rewritten in the form

$$1 < \Psi(\delta_n) \leq 1 + \gamma_1,$$

where

$$\Psi(\delta_n) = \left(\frac{\delta_n + p}{p}\right)^p \left(\frac{p-1}{\delta_n + (p-1)}\right)^{p-1} \quad \text{and} \quad \gamma_1 = \gamma / \det\{\mathbf{M}(\xi_n)\}.$$

Furthermore, for $\delta_n > 0$

$$\begin{aligned} \frac{\partial \Psi(\delta_n)}{\partial \delta_n} &= \frac{\partial}{\partial \delta_n}\left\{\left(\frac{\delta_n + p}{p}\right)^p \left(\frac{p-1}{\delta_n + (p-1)}\right)^{p-1}\right\} \\ &= \frac{(p-1)^{p-1}}{p^p} \frac{(\delta_n + p)^{p-1}\delta_n}{(\delta_n + p - 1)^p} \\ &> 0. \end{aligned}$$

It follows that $\Psi(\delta_n)$ is increasing continuous function. Therefore, Ψ^{-1} exists and is also continuous and increasing function (Bartel and Sherbert, 2000, page 152). Thus, we have

$$1 < \Psi(\delta_n) \leq 1 + \gamma_1 \quad \Rightarrow \quad 0 = \Psi^{-1}(1) < \delta_n \leq \Psi^{-1}(1 + \gamma_1). \tag{7.6}$$

It follows that for any $\gamma > 0$, we can find γ_1 such that for any $\varepsilon > 0$, we have

$$\Psi^{-1}(1 + \gamma_1) \leq \varepsilon. \tag{7.7}$$

Thus by (7.6) and (7.7), we can always find n^* which depends on ε such that for $n > n^*$

$$\bar{d}(\xi_n) - p = \delta_n \leq \varepsilon.$$

On the other hand, by the general equivalence theorem, $\bar{d}(\xi_n) - p = \delta_n \geq 0$ with equality if and only if ξ_n is D-optimal. By the assumption (7.2), there is a positive number ζ such that for any n

$$\bar{d}(\xi_n) - p = \delta_n \geq \zeta > 0. \tag{7.8}$$

Since ε is arbitrary, we can choose $\varepsilon < \zeta$. Then if we have $\delta_n \leq \varepsilon < \zeta$, we get a contradiction with (7.8), which proves the theorem. □

Remark 1. Since

$$\max_{x\in\chi}\det\{(\mathbf{X}_n'\mathbf{X}_n)^{j+1}\} \geq \det\{(\mathbf{X}_n'\mathbf{X}_n)^{j+1}\}|_{x=x_i} = \det\{(\mathbf{X}_n'\mathbf{X}_n)^{j}\},$$

the exchange algorithms never results in a decrease of the determinant of the information matrix $\mathbf{M}(\xi_n^j) = (\mathbf{X}_n'\mathbf{X}_n)^j/n$. Therefore,

$$\det\{\mathbf{M}(\xi_n^0)\} \leq \det\{\mathbf{M}(\xi_n^1)\} \leq \cdots \leq \det\{\mathbf{M}(\xi_n^j)\} \leq \cdots. \tag{7.9}$$

The sequence (7.9) is bounded above by $\det\{\mathbf{M}(\xi_n^*)\}$, where ξ_n^* is a D-optimal design. Thus, the sequence $\{\det\{\mathbf{M}(\xi_n^j)\}\}$ is monotonically convergent. Whether it actually converges to a D-optimal design remains an open question, although made plausible by numerical evidence. This will be discussed in the next section.

8 Empirical results

In this section, we explain and compare the modified Federov's algorithms. We consider the following rational regression model

$$\mathbf{E}(\mathbf{Y}_x) = \beta_1 + \frac{\beta_2}{1-0.2x} + \frac{\beta_3}{1+0.2x} + \frac{\beta_4}{1-0.4x} + \frac{\beta_5}{1+0.4x} + \frac{\beta_6}{1-0.6x} + \frac{\beta_7}{1+0.6x} + \frac{\beta_8}{1-0.8x} + \frac{\beta_9}{1+0.8x}.$$

Here

$$\mathbf{f}(x) = \left(1, \frac{1}{1-0.2x}, \frac{1}{1+0.2x}, \frac{1}{1-0.4x}, \frac{1}{1+0.4x}, \frac{1}{1-0.6x}, \frac{1}{1+0.6x}, \frac{1}{1-0.8x}, \frac{1}{1+0.8x}\right)'.$$

This example was also considered by Al Labadi and Zhen (2010). All algorithms are implemented in R, and the source code is available upon request from the author. We have considered 100 possible (candidate) points to be added/exchanged from the design region $[-1, 1]$. These candidate points are given by $x_i = -1 + 2i/99$, $i = 0, \ldots, 99$. We let the starting design for the two algorithms be the Chebyshev 9-point design. That is, $x_i = \cos((2i-1)\pi/18)$, $i = 1, \ldots, p = 9$ with equal weight $1/9$. Thus, the initial design is given by

$$\xi_9 = \left\{\begin{matrix} -0.9848, & -0.8660, & -0.6428, & -0.3420, & 0, & 0.3420, & 0.6428, & 0.8660, & 0.9848 \\ \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9}, & \frac{1}{9} \end{matrix}\right\}.$$

In what follows, to simplify the notations, the weights of the design points are omitted.

We consider first the modified Fedorov's algorithm. We compute $\mathbf{M}(\xi_9)$ and $\mathbf{M}^{-1}(\xi_9)$. Then the maximum value of the variance function $d(x, \xi_9)$ is 36.0783 and it occurs at $x = \pm 1.0000$. Since $\bar{d}(\xi_9) \neq 9$, by the general equivalence theorem, this design is not D-optimal. Then the two points $x = \pm 1.0000$ are added to the designs to get the new design ξ_{11}. We recalculate $\mathbf{M}(\xi_{11})$ as follows. First we find the best α that maximizes

$$\det\{\mathbf{M}(\xi_{11})\} = (1-2\alpha)^9 \det\left\{\mathbf{M}(\xi_9) + \frac{\alpha}{1-2\alpha}\mathbf{f}(-1)\mathbf{f}'(-1) + \frac{\alpha}{1-2\alpha}\mathbf{f}(1)\mathbf{f}'(1)\right\}.$$

The best α is 0.0850. Next we find $\mathbf{M}(\xi_{11})$, where

$$\mathbf{M}(\xi_{11}) = (1 - 2 \times 0.085)\mathbf{M}(\xi_9) + 0.0850\mathbf{f}(-1)\mathbf{f}'(-1) + 0.085\mathbf{f}(1)\mathbf{f}'(1).$$

The maximum variance is now 18.2583. Thus, the variance at the points $x = \pm 1.0000$ has been appreciably reduced by the addition of these two extra points. As $\bar{d}(\xi_{11}) \neq 9$, by the general equivalence theorem, this design is still not D-optimal. The two maxima of the curve $d(x, \xi_{11})$ are now $x = \pm 0.9394$. When these two points are added to the design ξ_{11}, we obtain ξ_{13}. We recalculate $\mathbf{M}(\xi_{13})$ as above. The maximum variance of the new design ξ_{13} is now 13.5945 and it occurs at $x = \pm 0.7576$. Clearly, this design is still not D-optimal. The process can be continued. Table 1 shows the construction of the design for 24 iterations.

Now we consider the modified exchange algorithm. To find the pair that will be exchanged, we compute $\max_{x_i \in \xi_9^1} \max_{x \in \chi} \det\{(\mathbf{X}_9'\mathbf{X}_9)^2\}$ which is achieved at ± 0.9848. Then we find new pair of the candidates points which makes $\det\{(\mathbf{X}_9'\mathbf{X}_9)^2\}$ as large as possible. The maximum value is found at $x = \pm 1.0000$. Thus, the pair ± 0.9848 is exchanged by ± 1.0000. The obtained design is

$$\xi_9^1 = \{\pm 1.0000, \pm 0.8660, \pm 0.6428, \pm 0.3420, 0\}.$$

Then we recompute $(\mathbf{X}_9'\mathbf{X}_9)^2$ and $\det\{(\mathbf{X}_9'\mathbf{X}_9)^2\}$ before exchanging the next pair of points. The largest value of Δ for this iteration is 2.5256. The variance function for the design ξ_9^2 is reduced to 30.4722. Since $\max_{x_i \in \xi_9^2} \max_{x \in \chi} \det\{(\mathbf{X}_9'\mathbf{X}_9)^3\}$ is achieved at ± 0.8660, this pair of points is exchanged by ± 0.9192. The new design is

$$\xi_9^2 = \{\pm 1.0000, \pm 0.9192, \pm 0.6428, \pm 0.3420, 0\}.$$

Again, we recompute $(\mathbf{X}_9'\mathbf{X}_9)^3$ and $\det\{(\mathbf{X}_9'\mathbf{X}_9)^3\}$. The largest value of Δ at this step is 1.16709. Since $\max_{x_i \in \xi_9^3} \max_{x \in \chi} \det\{(\mathbf{X}_9'\mathbf{X}_9)^4\}$ is achieved at ± 0.6428, this pair of points is exchanged by ± 0.7374. The new design is given by

$$\xi_9^3 = \{\pm 1.0000, \pm 0.9192, \pm 0.7374, \pm 0.3420, 0\}.$$

Table 1 *The modified Fedorov's sequential algorithm for constructing D-optimal design rational regression*

Iteration	n	x_{n+1}	x_{n+2}	α	$\bar{d}(\xi_n)$	$\det\{\mathbf{M}(\xi_n)\}$
0	9	−1.0000	1.0000	–	36.0783	5.9891×10^{-33}
1	11	−0.9394	0.9393	0.0850	18.2583	2.3229×10^{-32}
2	13	−0.7576	0.7576	0.0600	13.5945	3.6608×10^{-32}
3	15	−0.4343	0.4343	0.0450	12.1599	4.3719×10^{-32}
4	17	−0.0101	0.0101	0.0350	12.2229	4.8297×10^{-32}
5	19	−1.0000	1.0000	0.0150	11.8755	5.0601×10^{-32}
6	21	−0.9394	0.9394	0.0300	11.4372	5.5132×10^{-32}
7	23	−0.7576	0.7576	0.0300	10.9836	5.8845×10^{-32}
8	25	−0.4343	0.4343	0.0250	10.8837	6.1615×10^{-32}
9	27	−0.0101	0.0101	0.0250	11.367	6.4253×10^{-32}
10	29	−1.0000	1.0000	0.0150	11.0394	6.6025×10^{-32}
11	31	−0.9394	0.9394	0.0250	10.6065	6.9292×10^{-32}
12	33	−0.7576	0.7576	0.0200	10.6056	7.1533×10^{-32}
13	35	−0.4343	0.4343	0.0200	10.4409	7.3845×10^{-32}
14	37	−0.0101	0.0101	0.0200	10.287	7.5803×10^{-32}
15	39	−1.0000	1.0000	0.0100	10.3500	7.6471×10^{-32}
16	41	−0.9394	0.9394	0.0200	10.3887	7.8258×10^{-32}
17	43	−0.7576	0.7576	0.0200	10.4031	8.0193×10^{-32}
18	45	−0.4343	0.4343	0.0200	10.2798	8.2216×10^{-32}
19	47	−0.0101	0.0101	0.0150	10.0935	8.3953×10^{-32}
20	49	−1.0000	1.0000	0.0050	10.0026	8.4513×10^{-32}
21	51	−0.9394	0.9394	0.0150	9.9243	8.5661×10^{-32}
22	53	−0.7575	0.7575	0.0150	9.8433	8.6645×10^{-32}
23	55	−0.0101	0.0101	0.0100	10.0296	8.7479×10^{-32}

We recalculate $(\mathbf{X}_9'\mathbf{X}_9)^4$ and $\det\{(\mathbf{X}_9'\mathbf{X}_9)^4\}$. The largest value of Δ is now 0.93290. The value 0.93290 of Δ is still not close enough to zero, thus we continue the algorithm. The complete steps are summarized in Table 2.

Considering the modified Wynn algorithm (Al Labadi and Zhen, 2010, Table 1), it follows that the modified Fedorov's exchange algorithm is the fastest algorithm among the three modified algorithms, provided the same initial design. On the other hand, the modified Fedorov algorithm performs better than the modified Wynn algorithm in the first few iterations of applying the algorithm (the first 9 iterations in this example). When n gets large, then both algorithms behave similarly.

9 Concluding remarks

In this paper, we have described some refinements of Fedorov's sequential algorithm and Fedorov's exchange algorithm for constructing D-optimal designs. By

Table 2 *The modified Fedorov's exchange algorithm for constructing D-optimal design for rational regression*

Iteration j	$\pm x_i$	$\pm x$	$\bar{d}(\xi_9^j)$	$\max_{x\in\chi} \det\{(\mathbf{X}_9'\mathbf{X}_9)^j\}$	Δ
1	–	–	36.0783	2.3203×10^{-24}	–
2	±0.9848	±1.0000	30.4722	8.1805×10^{-24}	2.5256
3	±0.8660	±0.9192	20.642	1.7728×10^{-23}	1.1671
4	±0.6428	±0.7374	13.0356	3.3457×10^{-23}	0.9324
5	±0.3420	±0.4343	9.6633	4.7000×10^{-23}	0.3720
6	±0.9192	±0.9394	9.5787	4.8998×10^{-23}	0.0425
7	±0.7374	±0.7576	9.0198	5.1110×10^{-23}	0.0431
8	–	–	9.0198	5.111×10^{-23}	0.0000

the modified algorithms, we are able to perform multiple additions or exchanges simultaneously at each step. This will significantly reduce the computational time. Similar extensions to other existing algorithms, such as the k-exchange algorithm (Johnson and Nachtsheim, 1983), the kl-exchange algorithm (Atkinson and Donev, 1989), and the coordinate-exchange algorithm (Meyer and Nachtsheim, 1995), could be developed.

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