Monotonic convergence of a general algorithm for computing optimal designs

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Abstract

Monotonic convergence is established for a general class of multiplicative algorithms introduced by Silvey et al. (1978) for computing optimal designs. A conjecture of Titterington (1978) is confirmed as a consequence. Optimal designs for logistic regression are used as an illustration.

Keywords: A-optimality; auxiliary variables; c-optimality; D-optimality; experimental design; generalized linear models; multiplicative algorithm.

1 A general class of algorithms

Optimal experimental design (approximate theory) is a well-developed area and we refer to Kiefer (1974), Silvey (1980), Pázmán (1986), and Pukelsheim (1993) for general introduction and basic results. We consider computational aspects of optimal designs, focusing on a finite design space \( \mathcal{X} = \{x_1, \ldots, x_n\} \). Suppose the probability density or mass function of the response is specified as \( p(y|x; \theta) \), where \( \theta \) is the \( m \times 1 \) parameter of interest. Let \( A_i \) denote the \( m \times m \) expected Fisher information matrix from a unit assigned to \( x_i \) (the expectation is with respect to \( p(y|x_i, \theta) \)):

\[
A_i = E[s(\theta; y, x_i)s^\top(\theta; y, x_i)], \quad s(\theta; y, x_i) = \frac{\partial \log p(y|x_i, \theta)}{\partial \theta}.
\]

The moment matrix, as a function of the design measure \( w = (w_1, \ldots, w_n) \), is defined as

\[
M(w) = \sum_{i=1}^{n} w_i A_i,
\]

which is proportional to the Fisher information for \( \theta \) when the number of units assigned to \( x_i \) is proportional to \( w_i \). Here \( w \in \bar{\Omega} \), and \( \bar{\Omega} \) denotes the closure of \( \Omega = \{w : w_i > 0, \sum_{i=1}^{n} w_i = 1\} \).

Throughout we assume that \( A_i \) are well-defined and nonnegative definite (for fixed \( \theta \)). The set

\[
\Omega_+ \equiv \{w \in \bar{\Omega} : M(w) > 0 \text{ (positive definite)}\}
\]

is assumed nonempty. Our approach may conceivably extend to the case where \( M(w) \) is allowed singular, by using generalized inverses, although we do not pursue this here.

Given an optimality criterion \( \phi \), defined on positive definite matrices, the goal is to maximize \( \phi(M(w)) \) with respect to \( w \in \Omega_+ \). Typical optimality criteria include...
(i) the D-criterion $\phi_0(M) = \log \det(M)$,
(ii) the A-criterion $\phi_{-1}(M) = -tr(M^{-1})$,
(iii) more generally, the $p$th mean criterion $\phi_p(M) = -tr(M^p)$, $p < 0$, and
(iv) the c-criterion $\phi_c(M) = -c^\top M^{-1}c$, where $c$ is a nonzero constant vector.

(Our notation is mostly for convenience and may not correspond exactly to those of well-known texts.) Often only a linear combination $K^\top \theta$, e.g., a subvector of $\theta$, is of interest. Assuming invertibility, the Fisher information for $K^\top \theta$ is naturally defined as $(K^\top M^{-1}K)^{-1}$ (Pukelsheim, 1993). We may therefore consider the D- and A-criteria for $K^\top \theta$ defined respectively as

\[ \phi_{0,K}(M) = - \log \det(K^\top M^{-1}K); \]
\[ \phi_{-1,K}(M) = -tr(K^\top M^{-1}K). \]

(1)

The c-criterion is a special case of $\phi_{-1,K}(M)$. Motivations for such optimality criteria are well-known. For example, in a linear problem, the A-criterion seeks to minimize the sum of variances of the best linear unbiased estimators (BLUEs) for all coordinates of $w$, while the c-criterion seeks to minimize the variance of the BLUE for $c^\top \theta$. Similar interpretations (with asymptotic arguments) apply to nonlinear problems.

In general $M(w)$ also depends on the unknown parameter $\theta$, which complicates the definition of an optimality criterion. A simple solution is to maximize $\phi(M(w))$ with $\theta$ fixed at a prior guess $\theta^*$; this leads to local optimality (Chernoff 1953). Local optimality may be criticized for ignoring uncertainty in $\theta$. However, in a situation where real prior information is available, or where the dependence of $M$ on $\theta$ is weak, it is nevertheless a viable approach, and has been adopted routinely (see, for example, Li and Majumdar 2008). Henceforth we assume a fixed $\theta^*$ and suppress the dependence of $M$ on $\theta$. Possible extensions are mentioned in Section 5.

Optimal designs do not usually come in closed form. As early as Wynn (1972), Fedorov (1972) and Atwood (1973), and as late as Torsney (2007), Harman and Pronzato (2007), and Dette (2008), various procedures have been studied for numerical computation. We shall focus on the following multiplicative algorithm (Titterington 1976, 1978; Silvey 1978), which is specified through a power parameter $\lambda \in (0, 1]$.

**Algorithm I** Set $\lambda \in (0, 1]$ and $w^{(0)} \in \Omega$. For $t = 0, 1, \ldots$, compute

\[ w_i^{(t+1)} = w_i^{(t)} \frac{d_i(w^{(t)})}{n \sum_{j=1}^{n} w_j^{(t)} d_j(w^{(t)})}, \quad i = 1, \ldots, n, \]

where

\[ d_i(w) = tr(\phi'(M(w)) A_i), \quad \phi'(M) = \frac{\partial \phi(M)}{\partial M}. \]

(3)

Iterate until convergence.

We defer the discussion on convergence criteria until Section 4. For a heuristic explanation, observe that (2) is equivalent to

\[ w_i^{(t+1)} \propto w_i^{(t)} \left( \frac{\partial \phi(M(w))}{\partial w_i} \right)_{w=w^{(t)}}^\lambda, \quad i = 1, \ldots, n. \]

(4)

The value of $\partial \phi(M(w))/\partial w_i$ indicates the amount of gain in information, as measured by $\phi$, by a slight increase in $w_i$, the weight on the $i$th design point. So (4) can be seen as adjusting $w$ so that relatively more weight is placed on design points whose increased weight may result in a larger gain in $\phi$. 

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Algorithm I is remarkable in its generality. For example, little restriction is placed on the underlying model $p(y|x, \theta)$. Part of the reason, of course, is that we focus on Fisher information and local optimality, which essentially reduces the problem to a linear one.

There exists a large literature on Algorithm I and its relatives; see, for example, Titterington (1976, 1978), Silvey et al. (1978), Pázmány (1986), Fellman (1989), Pukelsheim and Torsney (1991), Torsney and Mandal (2006), Harman and Pronzato (2007), and Dette et al. (2008). One feature that has attracted much attention is that Algorithm I appears to be monotonic, i.e., $\phi(M(w^{(t)}))$ increases in $t$, at least in some special cases. For example, when $\phi = \phi_0$ (for D-optimality) and $\lambda = 1$, Titterington (1976) and Pázmány (1986) have shown monotonicity using clever probabilistic and analytic inequalities; see also Dette (2008) and Harman and Trnovská (2009). Algorithm I is also known to be monotonic for $\phi = \phi_{-1,K}$ as in (1), assuming $\lambda = 1/2$ and $A_i$ are rank-one (Fellman 1974; Torsney 1983). Monotonicity is important because convergence then holds under mild assumptions (see Section 4). Results in these special cases suggest a monotonic convergence theory for a broad class of $\phi$, which is also supported by numerical evidence presented in some of the references above.

2 Main result

We aim to state general conditions on $\phi$ that ensure that Algorithm I converges monotonically. As a consequence certain known theoretical results are unified and generalized, and one particular conjecture (Titterington 1978) is confirmed. Define

$$\psi(M) \equiv -\phi(M^{-1}), \quad M > 0.$$  

The functions $\phi$ and $\psi$ are assumed to be differentiable on positive definite matrices. Our conditions are conveniently stated in terms of $\psi$. As usual, for two symmetric matrices, $M_1 \leq (\leq) M_2$ means $M_2 - M_1$ is nonnegative (positive) definite.

- $\psi(M)$ is increasing:

$$0 < M_1 \leq M_2 \implies \psi(M_1) \leq \psi(M_2),$$

or, equivalently, $\psi'(M)$ is nonnegative definite for positive definite $M$.

- $\psi(M)$ is concave:

$$\alpha \psi(M_1) + (1 - \alpha) \psi(M_2) \leq \psi(\alpha M_1 + (1 - \alpha) M_2),$$

for $\alpha \in [0,1], M_1, M_2 > 0$. Equivalently,

$$\psi(M_2) \leq \psi(M_1) + \text{tr}(\psi'(M_1)(M_2 - M_1)), \quad M_1, M_2 > 0.$$  

Condition (5) is usually satisfied by any reasonable information criterion (Pukelsheim 1993). Also note that, if (5) fails, then $\partial \phi(M(w))/\partial w_i$ on the right hand side of (4) is not even guaranteed to be nonnegative. The real restriction is the concavity condition (6). For example, (6) is not satisfied by $\psi_p(M) = -\phi_p(M^{-1})$ (the $p$th mean criterion) when $p < -1$. (It is usually assumed that $\phi(M)$, rather than $\psi(M)$, is concave.) Nevertheless, (6) is satisfied by a wide range of criteria, including the commonly used D-, A- or c-criteria (see Cases (i) and (ii) in the illustration of the main result below).

Our main result is as follows.
Theorem 1 (General monotonicity). Assume (5) and (6). Assume that in iteration (2),
\[ M(w^{(t)}) > 0, \quad \phi'(M(w^{(t)})) \neq 0, \quad \text{and} \quad M(w^{(t+1)}) > 0. \]
Then
\[ \phi(M(w^{(t+1)})) \geq \phi(M(w^{(t)})). \]

In other words, under mild conditions that ensure that (2) is well-defined (specifically, the denominator in (2) is nonzero), (5) and (6) imply that (2) monotonically increases the criterion \( \phi \). Let us illustrate Theorem 1 with some examples. For simplicity, in (i)–(iv) we display formulae for \( \lambda = 1 \) only, although the discussion applies to all \( \lambda \in (0, 1] \).

(i) Take
\[ \phi_p(M) = \begin{cases} 
\log \det M, & p = 0; \\
-\text{tr}(M^p), & p \in [-1, 0).
\end{cases} \]
Then \( \psi_p(M) \equiv -\phi_p(M^{-1}) \) satisfies (5) and (6) (see Appendix A). By Theorem 1, Algorithm I is monotonic for \( \phi = \phi_p, \ p \in [-1, 0] \). This generalizes the previously known cases \( p = 0 \) and \( p = -1 \) (with particular values of \( \lambda \)). The iteration (2) reads
\[ w_i^{(t+1)} = w_i^{(t)} \frac{\text{tr}(M^{p-1}(w^{(t)})A_i)}{\text{tr}(M^p(w^{(t)}))}, \quad i = 1, \ldots, n. \]

(ii) More generally, given a full rank \( m \times r \) matrix \( K (r \leq m) \), consider
\[ \psi_{p,K}(M^{-1}) \equiv -\phi_{p,K}(M) = \begin{cases} 
\log \det(K^\top M^{-1}K), & p = 0; \\
\text{tr}((K^\top M^{-1}K)^{-p}), & p \in [-1, 0).
\end{cases} \]
Then \( \psi_{p,K}(M) \) satisfies (5) and (6) (the proof is the same as in Case (i)). By Theorem 1, Algorithm I is monotonic for \( \phi = \phi_{p,K}, \ p \in [-1, 0] \). The iteration (2) reads
\[ w_i^{(t+1)} = w_i^{(t)} \frac{\text{tr}(M^{-1}K(K^\top M^{-1}K)^{-p-1}K^\top M^{-1}A_i)}{\text{tr}((K^\top M^{-1}K)^{-p})} \bigg|_{M=M(w^{(t)})}. \tag{8} \]

(iii) In particular, taking \( r = 1, \ K = c \) (an \( m \times 1 \) vector) and \( p = -1 \) in Case (ii), we obtain that Algorithm I is monotonic for the \( c \)-criterion \( \phi_c \). The iteration (8) reduces to (compare with Fellman 1974)
\[ w_i^{(t+1)} = w_i^{(t)} \frac{c^\top M^{-1}(w^{(t)})A_i M^{-1}(w^{(t)})c}{c^\top M^{-1}(w^{(t)})c}, \quad i = 1, \ldots, n. \]

(iv) Consider another example of Case (ii), with \( p = 0, \ r = m - 1 \) and \( K = (0_r, I_r)^\top \). Henceforth \( 0_r \) denotes the \( r \times 1 \) vector of zeros, and \( I_r \) denotes the \( r \times r \) identity matrix. Assume \( A_i = x_i x_i^\top, \ x_i^\top = (1, z_i^\top) \) and \( z_i \) is \( (m - 1) \times 1 \). This corresponds to a D-optimal design problem for the linear model with intercept
\[ y|\theta \sim N(x^\top \theta, \sigma^2), \quad x^\top = (1, z^\top), \]
where the parameter is \( \theta = (\theta_0, \theta_1, \ldots, \theta_{m-1})^\top \) but interest centers on \( (\theta_1, \ldots, \theta_{m-1}) \), not \( \theta_0 \). Nevertheless, as far as the design measure \( w \) is concerned, the optimality criterion, \( \phi_{0,K}(M) \), coincides with \( \phi_0(M) \), i.e.,
\[ -\log \det(K^\top M^{-1}(w)K) = \log \det M(w). \]
After some algebra, (8) reduces to

\[ w_i^{(t+1)} = w_i^{(t)} \frac{(z_i - \bar{z})^\top M_{c}^{-1}(w^{(t)})(z_i - \bar{z})}{m-1}, \quad i = 1, \ldots, n, \]  

(9)

where

\[ \bar{z} = \sum_{i=1}^{n} w_i^{(t)} z_i; \quad M_{c}(w^{(t)}) = \sum_{i=1}^{n} w_i^{(t)} (z_i - \bar{z})(z_i - \bar{z})^\top. \]

Thus (9) satisfies \( \det M(w^{(t+1)}) \geq \det M(w^{(t)}) \).

Monotonicity of (9) has been conjectured since Titterington (1978), and considerable numerical evidence has accumulated over the years. Recently, extending the arguments of Pázmán (1986), Dette et al. (2008) have obtained results that come very close to resolving Titterington’s conjecture. Nevertheless, we have been unable to extend their arguments any further. Instead we prove the more general Theorem 1 using a different approach, and settle this conjecture as a consequence.

The proof of Theorem 1 is achieved by using a method of auxiliary variables. When a function \( f(w) \) (e.g., \(-\det M(w)\)) to be minimized is complicated, we introduce a new variable \( Q \) and a function \( g(w, Q) \) such that \( \min_Q g(w, Q) = f(w) \) for all \( w \), thus transforming the problem into minimizing \( g(w, Q) \) over \( w \) and \( Q \) jointly. Then we may use an iterative conditional minimization strategy on \( g(w, Q) \). This is inspired by the EM algorithm (Dempster et al. 1977; Meng and van Dyk 1997); in particular, see Csizsár and Tusnády’s [6] interpretation (see [30] for a related interpretation of the data augmentation algorithm).

In Section 3 we analyze Algorithm I using this strategy. Although attention is paid to the mathematics, our focus is on intuitively appealing interpretations, which may lead to further extensions of Algorithm I with the same desirable monotonicity properties. If the algorithm is monotonic, then convergence can be established under mild conditions (Section 4). Section 5 contains an illustration with locally optimal designs for generalized linear models.

3 Explaining the monotonicity

A key observation is that the problem of maximizing \( \phi(M(w)) \), or, equivalently, minimizing \( \psi(M^{-1}(w)) \) can be formulated as a joint minimization over both the design and the estimator. Specifically, let us compare the original Problem P1 with its companion P2. Throughout \( A^{1/2} \) denotes the symmetric nonnegative definite (SNND) square root of an SNND matrix \( A \).

**Problem P1:** Minimize \(-\phi(M(w)) \equiv \psi((\sum_{i=1}^{n} w_i A_i)^{-1}) \) over \( w \in \Omega \).

**Problem P2:** Minimize

\[ g(w, Q) \equiv \psi \left( Q \Delta_w Q^\top \right) \]

over \( w \in \Omega \) and \( Q \) (an \( m \times (mn) \) matrix), subject to \( QG = I_m \), where

\[ \Delta_w \equiv \text{Diag}(w_1^{-1}, \ldots, w_n^{-1}) \otimes I_m; \quad G \equiv (A_1^{1/2}, \ldots, A_n^{1/2})^\top. \]

Though not immediately obvious, P1 and P2 are equivalent, and this may be explained in statistical terms as follows. In (10), \( Q \Delta_w Q^\top \) is simply the variance matrix of a linear unbiased estimator, \( QY \), of the \( m \times 1 \) parameter \( \theta \) in the model

\[ Y = G\theta + \epsilon, \quad \epsilon \sim N(0, \Delta_w), \]
where $Y$ is the $(mn) \times 1$ vector of observations. The constraint $QG = I_m$ ensures unbiasedness. (Note that $G$ is full-rank since $M(w)$ is nonsingular by assumption.) Of course, the weighted least squares (WLS) estimator is the best linear unbiased estimator, having the smallest variance matrix (in the sense of positive definite ordering) and, by (5), the smallest $\psi$ for that matrix. It follows that, for fixed $w$, $g(w, Q)$ is minimized by choosing $QY$ as the WLS estimator:

$$g(w, \hat{Q}_{WLS}) = \inf_{QG = I_m} g(w, Q),$$

$$\hat{Q}_{WLS} = M^{-1}(w) \left( w_1A_1^{1/2}, \ldots, w_nA_n^{1/2} \right).$$

However, from (10) and (11) we get

$$g(w, \hat{Q}_{WLS}) = \psi(M^{-1}(w)).$$

That is, $P_2$ reduces to $P_1$ upon minimizing over $Q$.

Since $P_2$ is not immediately solvable, it is natural to consider the subproblems: (i) minimizing $g(w, Q)$ over $Q$ for fixed $w$, and (ii) minimizing $g(w, Q)$ over $w$ for fixed $Q$. Part (ii) is again formulated as a joint minimization problem. For a fixed $m \times (mn)$ matrix $Q$ such that $QG = I_m$, let us consider Problems $P_3$ and $P_4$.

**Problem P3:** Minimize $g(w, Q)$ as in (10) over $w \in \Omega$.

**Problem P4:** Minimize the function

$$h(\Sigma, w, Q) = \psi(\Sigma) + \text{tr} \left( \psi'(\Sigma) \left( Q\Delta_w Q^\top - \Sigma \right) \right)$$

over $w \in \Omega$ and the $m \times m$ positive-definite matrix $\Sigma$.

To relate $P_4$ to $P_3$, note that for fixed $w$ and $Q$, the concavity assumption (7) implies that

$$h(\Sigma, w, Q) \geq \psi \left( Q\Delta_w Q^\top \right)$$

with equality when $\Sigma = Q\Delta_w Q^\top$, i.e., Problem $P_4$ reduces to $P_3$ upon minimizing over $\Sigma$.

Since $P_4$ is not immediately solvable, it is natural to consider the subproblems: (i) minimizing $h(\Sigma, w, Q)$ over $\Sigma$ for fixed $w$ and $Q$, and (ii) minimizing $h(\Sigma, w, Q)$ over $w$ for fixed $\Sigma$ and $Q$. Part (ii), which amounts to minimizing

$$\text{tr} \left( \psi'(\Sigma) Q\Delta_w Q^\top \right) = \text{tr} \left( Q^\top \psi'(\Sigma) Q\Delta_w \right),$$

admits a closed-form solution: if we write $Q = (Q_1, \ldots, Q_n)$ where each $Q_i$ is $m \times m$, then $w_i^2$ should be proportional to $\text{tr}(Q_i^\top \psi'(\Sigma) Q_i)$. But algorithm I may not perform an exact minimization here; see (15).

Based on the above discussion, we can express Algorithm I as an iterative conditional minimization algorithm involving $w, Q$ and $\Sigma$. At iteration $t$, define

$$Q^{(t)} = (Q_1^{(t)}, \ldots, Q_n^{(t)});$$

$$Q_i^{(t)} = w_i^{(t)} M^{-1}(w_i^{(t)}) A_i^{1/2}, \quad i = 1, \ldots, n;$$

$$\Sigma^{(t)} = Q^{(t)} \Delta_w Q^{(t)\top} = M^{-1}(w^{(t)}).$$
Then we have
\[
\psi(M^{-1}(w^{(t)})) = g(w^{(t)}, Q^{(t)}) \quad \text{(by (12))}
\]
\[
= h(\Sigma^{(t)}, w^{(t)}, Q^{(t)}) \quad \text{(by (13))}
\]
\[
\geq h(\Sigma^{(t)}, w^{(t+1)}, Q^{(t)}) \quad \text{(see below) (15)}
\]
\[
\geq g(w^{(t+1)}, Q^{(t)}) \quad \text{(by (14), (10)) (16)}
\]
\[
\geq \psi(M^{-1}(w^{(t+1)})) \quad \text{(by (11), (12)). (17)}
\]

The choice of \(w^{(t+1)}\) leads to (15) as follows. After simple algebra, the iteration (2) becomes
\[
w^{(t+1)}_i = \frac{r_i^\lambda w_i^{-1-2\lambda}}{\sum_{j=1}^n r_j^\lambda w_j^{-1-2\lambda}}, \quad i = 1, \ldots, n,
\]
where
\[
w_i \equiv w_i^{(t)}, \quad r_i \equiv tr \left( Q_i^{(t)^T} \psi'(\Sigma^{(t)}) Q_i^{(t)} \right).
\]
Since \(0 < \lambda \leq 1\), Jensen’s inequality yields
\[
\left( \sum_{i=1}^n \frac{r_i}{w_i} \right)^{1-\lambda} \geq \sum_{i=1}^n w_i \left( \frac{r_i}{w_i} \right)^{1-\lambda}; \quad \left( \sum_{i=1}^n \frac{r_i}{w_i} \right)^{\lambda} \geq \sum_{i=1}^n \left( \frac{r_i}{w_i} \right)^{\lambda}.
\]
That is,
\[
\sum_{i=1}^n \frac{r_i}{w_i} \geq \left( \sum_{i=1}^n r_i^{1-\lambda} w_i^{2\lambda-1} \right) \left( \sum_{i=1}^n r_i^{\lambda} w_i^{1-2\lambda} \right).
\]
Hence
\[
tr \left( \psi'(\Sigma^{(t)}) Q^{(t)} \Delta_{w^{(t)}} Q^{(t)^T} \right) = \sum_{i=1}^n \frac{r_i}{w_i^{(t)}}
\]
\[
\geq \sum_{i=1}^n \frac{r_i}{w_i^{(t+1)}} = tr \left( \psi'(\Sigma^{(t)}) Q^{(t)} \Delta_{w^{(t+1)}} Q^{(t)^T} \right),
\]
which produces (15). Choosing \(\lambda = 1/2\), i.e., \(w_i^{(t+1)} \propto \sqrt{r_i}\), leads to exact minimization in (15); choosing \(\lambda = 1\) yields equality in (15). But any choice of \(w^{(t+1)}\) that decreases \(h(\Sigma^{(t)}, w, Q^{(t)})\) at (15) would have resulted in the desired inequality
\[
\psi(M^{-1}(w^{(t)})) \geq \psi(M^{-1}(w^{(t+1)})).
\]

We may allow \(\lambda\) to change from iteration to iteration, and monotonicity still holds, as long as \(\lambda \in (0, 1]\). See Silvey et al. (1978) and Fellman (1989) for investigations concerning the choice of \(\lambda\). Also note that we assume \(w_i^{(t)}, w_i^{(t+1)} > 0\) for all \(i\). This is not essential, however, because (i) the possibility of \(w_i^{(t)} = 0\) can be handled by restricting our analysis to all design points \(i\) such that \(w_i^{(t)} > 0\), and (ii) the possibility of \(w_i^{(t+1)} = 0\) can be handled by a standard limiting argument. Monotonicity holds as long as \(M(w^{(t)})\) and \(M(w^{(t+1)})\) are both positive definite, as noted in the statement of Theorem 1.
4 Global convergence

Let us review characterizations of optimal designs, commonly referred to as general equivalence theorems; see Kiefer and Wolfowitz (1960) and Whittle (1973).

**Theorem 2.** Assume the criterion $\phi$ is differentiable and concave. Define

$$d(w) \equiv \sum_{i=1}^{n} w_i d_i(w) = tr(\phi'(M(w))A_i),$$

where, as in (3), $d_i(w) \equiv tr(\phi'(M(w))A_i)$. Then for every $w^* \in \Omega_+$, the following are equivalent:

(a) $w^*$ maximizes $\phi(M(w))$ on $\Omega_+$;

(b) $d_i(w^*) \leq d_i(w)$ for all $i$;

(c) for all $i$, if $w_i^* \neq 0$ then $d_i(w^*) = d_i(w)$, and if $w_i^* = 0$ then $d_i(w^*) \leq d_i(w)$.

Theorem 2 suggests the following convergence criterion for Algorithm I: stop when

$$\max_{1 \leq i \leq n} d_i(w^{(t)}) \leq (1 + \delta) d(w^{(0)}),$$

(18)

for some small $\delta > 0$. Theorem 2 also plays an important role in the proof of our main convergence result (Theorem 3). Of course, the driving force behind Theorem 3 is monotonicity (Theorem 1).

**Theorem 3** (Global convergence). Denote the mapping (2) by $T$.

(a) Assume

$$\phi'(M(w)) \geq 0; \quad \phi'(M(w))A_i \neq 0, \quad w \in \Omega_+, \ i = 1, \ldots, n.$$

(b) Assume (2) is strictly monotonic, i.e.,

$$w \in \Omega_+, \ Tw \neq w \implies \phi(M(Tw)) > \phi(M(w)).$$

(19)

(c) Assume $\phi$ is strictly concave and $\phi'$ is continuous on positive definite matrices.

(d) Assume that, if $M$ (a positive definite matrix) tends to $M^*$ such that $\phi(M)$ increases monotonically, then $M^*$ is nonsingular.

Let $w^{(t)}$ be generated by (2) with $w_i^{(0)} > 0$ for all $i$. Then

(i) all limit points of $w^{(t)}$ are global maxima of $\phi(M(w))$, and

(ii) as $t \to \infty$, $\phi(M(w^{(t)}))$ increases monotonically to $\sup_{w \in \Omega_+} \phi(M(w))$.

The proof of Theorem 3 is somewhat subtle. Standard arguments (see Lemma 1 in Appendix B) show that all limit points of $w^{(t)}$ are fixed points of the mapping $T$. This alone does not imply convergence to a global maximum, however, because there often exist sub-optimal fixed points on the boundary of $\Omega$. (Global maxima occur routinely on the boundary also.) Our goal is therefore to rule out possible convergence to such sub-optimal points; Appendix B presents the details. We shall comment on Conditions (a)–(d).

Condition (a) ensures that starting with $w^{(0)} \in \Omega_+$, all iterations are well-defined. Moreover, if $w_i^{(0)} > 0$ for all $i$, then $w_i^{(t)} > 0$ for all $t$ and $i$. This highlights the following basic idea. In order to converge to a global maximum $w^*$, the starting value $w^{(0)}$ must assign positive weight to every support point of $w^*$. Such a requirement is not necessary for monotonicity. On the
other hand, assigning weight to non-supporting points of $w^*$ tends to slow the algorithm down. Hence methods that quickly eliminate non-optimal support points are valuable (Harman and Pronzato, 2007).

Condition (b) simply says that unless $w$ is a fixed point, the mapping $T$ should produce a better solution. Let us assume (5), (7) and Condition (a), so that Theorem 1 applies. Then, by checking the equality condition in (15), it is easy to see that Condition (b) is satisfied if $0 < \lambda < 1$. (The argument leading to (19) technically assumes that all coordinates of $w$ are nonzero, but we can apply it to the appropriate subvector of $w$.) If $\lambda = 1$, then (15) reduces to an equality. However, by checking the equality conditions in (16) and (17), we can show that Condition (b) is satisfied if $0 < \lambda < 1$. (The argument leading to (19) technically assumes that all coordinates of $w$ are nonzero, but we can apply it to the appropriate subvector of $w$.)

Conditions (c) and (d) are technical requirements that concern $\phi$ alone. Condition (c) ensures uniqueness of the optimal moment matrix, which simplifies the analysis. Condition (d) ensures that positive definiteness of $M(w)$ is maintained in the limit. Conditions (c) and (d) are satisfied by $\phi = \phi_p$ with $p \leq 0$, for example.

Let us mention a typical example of Theorem 3.

**Corollary 1.** Assume $A_i \neq 0$, $w_i^{(0)} > 0$, $i = 1, \ldots, n$, and $M(w^{(0)}) > 0$. Then the conclusion of Theorem 3 holds for Algorithm I with $\phi = \phi_0$.

**Proof.** Conditions (a), (c) and (d) are readily verified. Condition (b) is satisfied by (20) and (21). The claim follows from Theorem 3.

A more specialized example concerns (9).

**Proposition 1.** Assume that $X = (x_1, \ldots, x_n)$ as in (9) has rank $m$, and that $w_i^{(0)} > 0$ for all $i$. Then the conclusion of Theorem 3, with $\phi = \phi_0$, holds for the iteration (9).

The iteration (9) technically does not satisfy the assumptions of Theorem 3. For example, we do not have $w_i^{(t+1)} > 0$ even if $w_i^{(t)} > 0$ for all $i$. However, inspection of (9) shows that $w_i^{(t+1)}$ is set to zero only when $z_i = \bar{z}$, in which case it can be shown that an optimal design need not include $x_i$ as a support point, i.e., $x_i$ is safely eliminated. Proposition 1 can be established by following the proof of Theorem 3 step by step, rather than appealing to Theorem 3 directly. We omit the details.

### 5 Remarks and illustrations

The literature abounds with numerical examples of Algorithm I and its relatives. There are several reasons for such wide interest. Similar to the EM algorithm, Algorithm I is simple, easy to implement, and monotonically convergent for a large class of optimality criteria (although this was not proved in the present generality). Algorithm I is known to be slow sometimes. But it serves as a foundation upon which more effective variants can be built (see, e.g., Harman and Pronzato 2007, and Dette et al. 2008). While solving the conjectured monotonicity of (9) holds mathematical interest, our main contribution is a way of interpreting such algorithms as
optimization on augmented spaces. This opens up new possibilities in constructing algorithms with the same desirable monotonic convergence properties.

As a numerical example, consider the logistic regression model

$$p(y|x, \theta) = \frac{\exp(yx^\top \theta)}{1 + \exp(x^\top \theta)}, \quad y = 0, 1.$$  

The expected Fisher information for $\theta$ from a unit assigned to $x_i$ is

$$A_i = x_i \frac{\exp(x_i^\top \theta)}{(1 + \exp(x_i^\top \theta))^2} x_i^\top.$$  

We compute locally optimal designs with prior guess $\theta^* = (1, 1)^\top$ ($m = 2$), and design spaces

$$\mathcal{X}_1 = \{ x_i = (1, i/20)^\top, \ i = 1, \ldots, 20 \};$$

$$\mathcal{X}_2 = \{ x_i = (1, i/10)^\top, \ i = 1, \ldots, 30 \}.$$  

The expected Fisher information for $\theta$ from a unit assigned to $x_i$ is

$$A_i = x_i \frac{\exp(x_i^\top \theta)}{(1 + \exp(x_i^\top \theta))^2} x_i^\top.$$  

The design criteria considered are $\phi_0$ (for D-optimality) and $\phi_{-2}$. We use Algorithm I with $\lambda = 1$, starting with equally weighted designs.

For $\phi_0$, Corollary 1 guarantees monotonic convergence. This is illustrated by Figure 1, the first row, where $\phi_0 = \log \det M(w)$ is plotted against iteration $t$. Using the convergence criterion (18) with $\delta = 0.0001$, the number of iterations until convergence is 93 for $\mathcal{X}_1$ and 2121 for $\mathcal{X}_2$. The actual locally D-optimal designs are $w_1 = w_{20} = 0.5$ for $\mathcal{X}_1$ and $w_1 = w_{23} = 0.5$ for $\mathcal{X}_2$, as can be verified using the general equivalence theorem. This simple example serves to illustrate both the monotonicity of Algorithm I (when Theorem 1 applies) and its potential slow convergence.

For $\phi_{-2}$, although Algorithm I can be implemented just as easily, Theorem 1 does not apply, because the concavity condition (7) no longer holds. Indeed, Algorithm I (with $\lambda = 1$) is not monotonic, as is evident from Figure 1, the second row, where $\phi_{-2} = -\text{tr}(M^{-2}(w))$ is plotted against iteration $t$. This shows the potential danger of using Algorithm I when monotonicity is not guaranteed. It seems worthwhile to investigate modifications that may again lead to monotonic convergence in such situations.

We have focused on local optimality criteria. An alternative, *Bayesian optimality* (Chaloner and Larntz, 1989; Chaloner and Verdinelli, 1995), seeks to maximize the expected value of $\phi(M(\theta; w))$ over a prior distribution $\pi(\theta)$. The notation $M(\theta; w)$ emphasizes the dependence of the moment matrix on the parameter $\theta$. It would be worthwhile to extend our strategy in Section 3 to Bayesian optimality, and we plan to report both theoretical and empirical evaluations of such extensions in future work.

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**Appendix A: Details of Case (i)**

We only verify (6), since (5) is easy. For $\psi_p(M) = \text{tr}(M^{-p})$, $p \in [-1, 0)$, (6) holds because the function $f(x) = x^{-p}, \ x \in [0, \infty), \ p \in [-1, 0)$, is operator concave (Bhatia 1997, Chapter V). For
Figure 1: Values of $\phi_0 = \log \det M$ (row 1) and $\phi_{-2} = -tr(M^{-2})$ (row 2) for Algorithm I with design spaces $X_1$ (left) and $X_2$ (right).
ψ₀(M) = \log \det M, a simple proof of (6) is to choose an m × m invertible matrix U such that
\[ U^T M_1 U = \text{Diag}(a_1, \ldots, a_m); \quad U^T M_2 U = \text{Diag}(b_1, \ldots, b_m). \]
Then (6) reduces to
\[ \alpha \sum_{i=1}^{m} \log a_i + (1 - \alpha) \sum_{i=1}^{m} \log b_i \leq \sum_{i=1}^{m} \log(\alpha a_i + (1 - \alpha)b_i), \]
which holds by Jensen’s inequality.

**Appendix B: Proof of Theorem 3**

**Lemma 1.** Any limit point \( w^* \) of \( w^{(t)} \) is a fixed point of \( T \), i.e., \( Tw^* = w^* \).

**Proof.** Let \( w^{(t_j)} \) be a subsequence converging to \( w^* \). By Theorem 1 and Condition (d), \( M(w^*) \) is positive definite, i.e., \( w^* \in \Omega_+ \). Moreover, since both \( T \) and the function \( \phi(M(\cdot)) \) are continuous on \( \Omega_+ \), we have
\[ \phi(M(w^*)) = \lim_{j \to \infty} \phi(M(w^{(t_j)})) = \lim_{j \to \infty} \phi(M(w^{(t_j+1)})) = \phi(M(Tw^*)), \]
where the two limits are equal by monotonicity. From Condition (b) we deduce that \( Tw^* = w^* \).

**Lemma 2.** Suppose \( w^* \) is a limit point of \( w^{(t)} \), and define \( S_+ = \{ w \in \Omega_+ : w_i^* = 0 \implies w_i = 0 \} \), i.e., \( S_+ \) collects all \( w \) that are absolutely continuous with respect to \( w^* \) and satisfy \( M(w) > 0 \). Then we have
\[ \phi(M(w^*)) = \sup_{w \in S_+} \phi(M(w)); \quad \phi(M(\hat{w})) = \sup_{w \in S_+} \phi(M(w)) \implies M(\hat{w}) = M(w^*). \]  

**Proof.** By Lemma 1, \( w^* \) is a fixed point of \( T \). That is,
\[ w_i^* \neq 0 \implies \text{tr}(\phi'(M(w^*))A_i) = \text{tr}(\phi'(M(w^*)))M(w^*). \]
By Theorem 2, \( w^* \) maximizes \( \phi(M(w)) \) on \( S_+ \), and (22) is proved. The implication (23) holds because we assume \( \phi(\cdot) \) is strictly concave (Condition (c)).

**Lemma 3.** The sequence \( M(w^{(t)}) \) has finitely many limit points.

**Proof.** Since \( M(\cdot) \) is continuous, any limit point of \( M(w^{(t)}) \) is of the form \( M(w^*) \) for some limit point \( w^* \) of \( w^{(t)} \). By Lemma 2, \( M(w^*) \) is the unique maximizer of \( \phi(M) \) among all \( M > 0 \) that can be written as \( M = M(w) \) with \( w \ll w^* \). Depending on which coordinates of \( w^* \) are zero, there are fewer than \( 2^n \) such “degenerate maximizers”.

**Lemma 4.** The limit \( M_\infty \equiv \lim_{t \to \infty} M(w^{(t)}) \) exists.
Proof. Assume \( M(w(t)) \) has \( L < \infty \) limit points, and let \( B_i, i = 1, \ldots, L \), be non-intersecting balls (neighborhoods) centered on these. We know \( L \geq 1 \) because \( M(w(t)) \) is bounded; the choice of a metric is immaterial. Again by boundedness, for large enough \( t \), each \( M(w(t)) \) belongs to exactly one of \( B_i \). Assume \( L \geq 2 \), i.e., \( M(w(t)) \) does not converge. Then there exists a subsequence such that \( M(w(t_j)), M(w(t_j+1)) \) always belong to different \( B_i \). By passing through a sub-subsequence if necessary, we may assume \( w(t_j) \to w^* \); by Lemma 1, \( w(t_j+1) \to w^* \). It follows that \( M(w(t_j)) \to M(w^*) \) and \( M(w(t_j+1)) \to M(w^*) \), which contradicts the assumption of distinct neighborhoods.

Lemma 5. The limit \( M_\infty \) as defined in Lemma 4 satisfies

\[
\phi(M_\infty) = \sup_{w \in \Omega_+} \phi(M(w)).
\]

Proof. Let us check the conditions of the general equivalence theorem, i.e.,

\[
tr(\phi'(M_\infty)A_i) \leq tr(\phi'(M_\infty)M_\infty), \quad i = 1, \ldots, n.
\]

Suppose this fails for \( i = 1 \), say, then by Lemma 4 there exists \( \delta > 0 \) such that for sufficiently large \( t \), we have

\[
tr \left( \phi'(M(w(t)))A_1 \right) > (1 + \delta)tr \left( \phi'(M(w(t)))M(w(t)) \right).
\]

It follows from the definition of \( T \) that

\[
\frac{w_1^{(t+1)}}{w_1^{(t)}} > (1 + \delta) \frac{\left( \sum_{i=1}^{n} w_i d_i \right)^{\lambda}}{\sum_{i=1}^{n} w_i d_i^\lambda},
\]

where \( d_i = tr(\phi'(M(w(t)))A_i) \). However, the right hand side of (24) is at least \( (1 + \delta)^\lambda \) due to Jensen’s inequality. That is,

\[
w_1^{(t+1)} > (1 + \delta)^\lambda w_1^{(t)}
\]

for all \( t \) large enough, which contradicts the obvious constraint \( 0 < w_1^{(t)} \leq 1 \).

Theorem 3 then follows from Lemma 5.

References


