

GENERALIZED MINIMUM ABERRATION AND DESIGN EFFICIENCY FOR NONREGULAR FRACTIONAL FACTORIAL DESIGNS

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Abstract: Tang and Deng (1999) proposed a generalized minimum aberration criterion (GMA) as a natural extension of the minimum aberration criterion (MA) from regular to nonregular designs. While MA was defined for regular designs only, GMA applies to both regular and nonregular designs. In this paper, we investigate the relationship between GMA and some model-dependent efficiency criteria, and show that GMA is supported by these criteria. An extensive evaluation of designs with 20 runs and 5 factors shows that the GMA criterion can be used to classify and rank-order these designs. Empirical studies also demonstrate that the GMA ranking is consistent with those obtained by using other model-dependent efficiency criteria.

Key words and phrases: D_f -criterion, estimation capacity, regular design, super-saturated design.

1. Introduction

The most commonly used designs for factorial experiments are two-level regular fractional factorial designs. Under the hierarchical assumption that lower-order effects are more important than higher-order effects and that effects of the same order are equally important, a minimum aberration (MA) design is preferred (Fries and Hunter (1980)). One drawback of using a regular two-level design is that its run size must be a power of 2. On the other hand, nonregular designs are much more abundant. For example, Hadamard matrices of order n can be used to construct orthogonal main-effect plans of size n . Recall that a Hadamard matrix \mathbf{H} of order n is a square matrix with ± 1 entries such that $\mathbf{H}'\mathbf{H} = n\mathbf{I}$. Such a matrix can be normalized so that all the entries in the first column are equal to 1. Taking any m columns other than the first, one obtains an n -run orthogonal main-effect plan for m factors.

Deng and Tang (1999) proposed a generalized minimum aberration criterion, a natural extension of MA from regular to nonregular designs. A simpler version, called minimum G_2 aberration, was proposed by Tang and Deng (1999). When applied to regular designs, both versions are the same as MA. Cheng, Steinberg

and Sun (1999) justified the MA criterion by showing that it is a good surrogate for model-robustness. In this paper, a similar study is carried out for generalized minimum aberration. By drawing a connection with some traditional design efficiency criteria, one can show that generalized minimum aberration is supported by these model-dependent criteria. For simplicity, we concentrate on the study of minimum G_2 aberration. In the rest of the paper, by generalized minimum aberration (GMA) we mean minimum G_2 aberration.

In Section 2, we review and comment on the GMA criterion. A connection with partial aliasing is discussed. In Section 3, a heuristic argument is given to show that GMA is a good surrogate for some classical design efficiency criteria. In Section 4, we perform an empirical study of designs with 20 runs and 5 factors constructed from Hadamard matrices. The empirical study demonstrates that the GMA ranking is very consistent with those obtained by using other model-dependent efficiency criteria.

2. Generalized Minimum Aberration

An n -run design d for m two-level factors can be represented by an $n \times m$ matrix of 1's and -1 's, where each column corresponds to a factor (or its main effect) and each row represents a factor-level combination. We denote such a matrix by $\mathbf{X}(d)$. The interactions are then represented by componentwise products of columns of $\mathbf{X}(d)$. Specifically, for $1 \leq s \leq m$ and any s -subset $S = \{j_1, \dots, j_s\}$ of $\{1, \dots, m\}$, let $\mathbf{x}_S(d)$ be the componentwise product of the j_1 th, \dots , and j_s th columns of $\mathbf{X}(d)$. Then $\mathbf{x}_S(d)$ represents a main effect when $s = 1$ and the interaction of factors j_1, \dots, j_s if $s \geq 2$. For a subset S of $\{1, \dots, m\}$, we denote the cardinality of S by $|S|$.

Define $j_S(d)$ as the sum of all the entries of $\mathbf{x}_S(d)$, and denote $|j_S(d)|$ by $J_S(d)$: $j_S(d) = \sum_{i=1}^n x_{ij_1}(d), \dots, x_{ij_s}(d)$, $J_S(d) = |j_S(d)|$, where $x_{ij}(d)$ is the (i, j) th entry of $\mathbf{X}(d)$. Let $B_s(d) = n^{-2} \sum_{S:|S|=s} [j_S(d)]^2$. The GMA criterion proposed by Tang and Deng (1999) is to sequentially minimize $B_1(d), B_2(d), \dots, B_m(d)$.

Recently, Tang (2001) showed that a design d is uniquely determined by the $j_S(d)$ values. A key identity derived in his paper implies that

$$n^{-1} \mathbf{1}_n = \sum_{S: S \subset \{1, \dots, m\}} [n^{-1} j_S(d)] [2^{-m} \mathbf{x}_S(d)], \quad (2.1)$$

where $\mathbf{1}_n$ is the $n \times 1$ vector of ones. Then for any $T \subset \{1, \dots, m\}$, by taking the componentwise product of $\mathbf{x}_T(d)$ with both sides of (2.1), we obtain

$$n^{-1} \mathbf{x}_T(d) = \sum_{S: S \subset \{1, \dots, m\}} [n^{-1} j_S(d)] [2^{-m} \mathbf{x}_S(d) \odot \mathbf{x}_T(d)],$$

where $\mathbf{x}_S(d) \odot \mathbf{x}_T(d)$ is the componentwise product of $\mathbf{x}_S(d)$ and $\mathbf{x}_T(d)$. It is easy to see that for any two subsets S and T of $\{1, \dots, m\}$, $\mathbf{x}_S(d) \odot \mathbf{x}_T(d) = \mathbf{x}_{S \Delta T}(d)$, where $S \Delta T = (S \cup T) \setminus (S \cap T)$, with $\mathbf{x}_\emptyset(d)$ being the vector of ones. Therefore

$$n^{-1}\mathbf{x}_T(d) = \sum_{S: S \subset \{1, \dots, m\}} [n^{-1}j_S(d)][2^{-m}\mathbf{x}_{S \Delta T}(d)]. \quad (2.2)$$

Equation (2.2) shows how a given factorial effect is aliased with other effects under design d . For regular designs, each $n^{-1}j_S(d)$ is 1, -1 or 0; so (2.2) is the usual method of determining the aliasing structure from the defining relation of the design. For nonregular designs, $|n^{-1}j_S(d)|$ can be strictly between 0 and 1, leading to so-called partial aliasing. The quantities $n^{-1}j_S(d)$ are the coefficients in this partial aliasing. GMA is consistent with the belief that aliasing among lower-order effects is less desirable.

The GMA criterion was originally proposed for designs constructed from Hadamard matrices, but clearly this criterion applies to all designs, orthogonal or not. We also point out that GMA can be used to discriminate among supersaturated designs. When applied to supersaturated designs, $B_2(d)$ is equivalent to the $E(s^2)$ -criterion proposed by Booth and Cox (1962). One can apply the GMA criterion to supersaturated designs as a refinement of the $E(s^2)$ -criterion. This approach provides a nice unification covering regular, nonregular, and supersaturated designs under a single umbrella.

In fact, B_2 is related to the so-called (M.S)-criterion (Eccleston and Hedayat (1974)), which has long been advocated in the optimal design literature as a good surrogate for such traditional optimality criteria as the D- and A-criteria. For example, consider a simple linear model $\mathbf{y} = \mathbf{X}\theta + \epsilon$, where θ is a vector of unknown parameters, ϵ is a vector of uncorrelated and homoscedastic random errors, and the design matrix \mathbf{X} is at the experimenter's disposal. A design is called D-optimal if it maximizes $\det(\mathbf{X}'\mathbf{X})$, and is (M.S)-optimal if it maximizes $\text{tr}(\mathbf{X}'\mathbf{X})$ and minimizes $\text{tr}[(\mathbf{X}'\mathbf{X})^2]$ among those which maximize $\text{tr}(\mathbf{X}'\mathbf{X})$. The (M.S)-criterion is much easier to deal with computationally, and is known to produce highly efficient, if not optimal, designs under many optimality criteria including the D-criterion; see Cheng (1996). When $\text{tr}(\mathbf{X}'\mathbf{X})$ is a constant, as in applications to two-level factorial designs where all the entries of \mathbf{X} are 1 or -1 , the (M.S)-criterion reduces to the minimization of $\text{tr}[(\mathbf{X}'\mathbf{X})^2]$. For main-effect plans, this is the same as to minimize B_2 . That minimizing $\text{tr}[(\mathbf{X}'\mathbf{X})^2]$ leads to efficient main-effect plans has been well documented in the optimal design literature. The GMA criterion can be viewed as an extension to situations where some interactions are present, as will be discussed in the next section.

In the rest of the paper, we shall assume that the two levels are equireplicated for each factor (so the run size is even). This implies that $B_1(d)$ is equal to zero.

3. Design Efficiency and GMA

Cheng, Steinberg and Sun (1999) provided some insight into minimum aberration and justified this criterion by demonstrating that it is a good surrogate for some model-robustness criteria. It is natural to investigate the relationship of GMA to “model robustness” of nonregular designs in the spirit of Cheng, Steinberg and Sun (1999). For simplicity, let us restrict to the situation where (i) the main effects are of primary interest and their estimates are required and (ii), the experimenter would like to have as much information about two-factor interactions as possible, under the assumption that three-factor and higher-order interactions are negligible.

One model-robustness criterion considered in Cheng, Steinberg and Sun (1999) is estimation capacity. For any $1 \leq f \leq \binom{m}{2}$, define the estimation capacity $E_f(d)$ of a regular 2^{m-q} design d as the total number of models containing all the main effects and f two-factor interactions that can be entertained by d . It is desirable to have $E_f(d)$ as large as possible (here one can think of f as the number of active two-factor interactions). Cheng, Steinberg and Sun (1999) showed that the minimum aberration criterion tends to produce designs with maximum $E_f(d)$, especially for small f 's.

One important difference between regular and nonregular designs is that under a regular design, as long as the factorial effects are estimable, full efficiency is achieved, but for nonregular designs, in addition to estimability, efficiency is also an issue due to complicated partial aliasing. In Cheng, Steinberg and Sun (1999), it is enough to consider the maximization of the number of estimable models. Their definition of maximum estimation capacity can be carried over to nonregular designs without modification, but will not be adequate since efficiencies are not addressed.

As in the original formulation of maximum estimation capacity, suppose there are f active two-factor interactions. Let \mathcal{P} consist of all the $\binom{m}{2}$ subsets of size two of $\{1, \dots, m\}$. Then the f active two-factor interactions correspond to an f -subset of \mathcal{P} , say \mathcal{F} . Under a two-level design d with m factors and n runs, we have the following linear model:

$$\mathbf{y} = \mu \mathbf{1}_n + \mathbf{X}(d)\beta_1 + \mathbf{Y}_{\mathcal{F}}(d)\beta_2 + \epsilon,$$

where \mathbf{y} is the $n \times 1$ vector of observations, μ is an unknown parameter representing the general mean, $\mathbf{X}(d)$ is as defined in Section 2, β_1 is the $m \times 1$ vector of main effects, $\mathbf{Y}_{\mathcal{F}}(d)$ is an $n \times f$ matrix consisting of the f columns $\mathbf{x}_S(d)$, where $S \in \mathcal{F}$, β_2 is the $f \times 1$ vector of active two-factor interactions, and ϵ is an $n \times 1$ random vector such that $E(\epsilon) = \mathbf{0}$ and $\text{cov}(\epsilon) = \sigma^2 \mathbf{I}_n$. Let $\mathbf{X}_{\mathcal{F}}(d) = [\mathbf{1}_n; \mathbf{X}(d);$

$\mathbf{Y}_{\mathcal{F}}(d)$]. Then the information matrix per observation of d is

$$\mathbf{M}_{\mathcal{F}}(d) = \frac{1}{n} \mathbf{X}_{\mathcal{F}}(d)' \mathbf{X}_{\mathcal{F}}(d) = \begin{bmatrix} 1 & 0 & \frac{1}{n} \mathbf{1}'_n \mathbf{Y}_{\mathcal{F}}(d) \\ 0 & \frac{1}{n} \mathbf{X}(d)' \mathbf{X}(d) & \frac{1}{n} \mathbf{X}(d)' \mathbf{Y}_{\mathcal{F}}(d) \\ \frac{1}{n} \mathbf{Y}_{\mathcal{F}}(d)' \mathbf{1}_n & \frac{1}{n} \mathbf{Y}_{\mathcal{F}}(d)' \mathbf{X}(d) & \frac{1}{n} \mathbf{Y}_{\mathcal{F}}(d)' \mathbf{Y}_{\mathcal{F}}(d) \end{bmatrix}. \quad (3.1)$$

The usual D-criterion seeks to maximize $\det(\mathbf{M}_{\mathcal{F}}(d))$. When it is unknown which f two-factor interactions are active, to evaluate a design, one may consider its average performance over all possible models with f two-factor interactions. This suggests the maximization of the average of $\det(\mathbf{M}_{\mathcal{F}}(d))$ over all $\binom{F}{f}$ f -subsets \mathcal{F} of \mathcal{P} , where $F = \binom{m}{2}$. We denote this average D-criterion by D_f .

It is convenient to think of \mathcal{F} as a random sample of size f from \mathcal{P} . Then we may write D_f as $D_f(d) = E_{\mathcal{F}}[\det(\mathbf{M}_{\mathcal{F}}(d))]$, where $E_{\mathcal{F}}$ denotes the expectation with respect to the random sampling of \mathcal{F} from \mathcal{P} .

However, $D_f(d)$ is difficult to calculate. Since minimizing $\text{tr}[(\mathbf{M}_{\mathcal{F}}(d))^2]$ is a good surrogate for maximizing $\det(\mathbf{M}_{\mathcal{F}}(d))$, we expect a design that minimizes $E_{\mathcal{F}}\{\text{tr}[(\mathbf{M}_{\mathcal{F}}(d))^2]\}$ to perform very well under the D_f -criterion. The calculation of $E_{\mathcal{F}}\{\text{tr}[(\mathbf{M}_{\mathcal{F}}(d))^2]\}$ is considerably easier, thus providing a simple and good surrogate for the D_f -criterion. Since all the diagonal entries of $\mathbf{M}_{\mathcal{F}}(d)$ are equal to 1, minimizing $E_{\mathcal{F}}\{\text{tr}[(\mathbf{M}_{\mathcal{F}}(d))^2]\}$ is the same as minimizing $E_{\mathcal{F}}\{\text{sum of squares of all off-diagonal entries of } \mathbf{M}_{\mathcal{F}}(d)\}$. For simplicity, we denote this last quantity as $S_f^2(d)$.

The following proposition shows that $S_f^2(d)$ is a linear combination of $B_2(d)$, $B_3(d)$ and $B_4(d)$ with decreasing weights.

Proposition 1. *Let d be an n -run design for m two-level factors such that the two levels are equireplicated for each factor. Let $F = \binom{m}{2}$ and f be any positive integer such that $f \leq F$. Then we have $S_f^2(d) = \alpha_2 B_2(d) + \alpha_3 B_3(d) + \alpha_4 B_4(d)$, where $\alpha_2 = 2\left[1 + \frac{f}{F} + \frac{f(f-1)}{F(F-1)}(m-2)\right]$, $\alpha_3 = 6\frac{f}{F}$ and $\alpha_4 = 6\frac{f(f-1)}{F(F-1)}$.*

The proof of Proposition 1 can be found in the Appendix. Proposition 1 shows that $S_f^2(d)$ depends only on m , f , $B_2(d)$, $B_3(d)$ and $B_4(d)$. Comparing α_2 , α_3 and α_4 , we see that if f is small relative to F (i.e., only a small number of two-factor interactions are expected to be active), then $B_2(d)$ carries a heavier weight than $B_3(d)$, which in turn has more influence on $S_f^2(d)$ than $B_4(d)$. Thus for small f , we expect the ranking of designs based on GMA to be quite consistent with that based on $S_f^2(d)$. The GMA criterion thus provides a good surrogate for D_f . The degree of consistency depends on f , the number of two-factor interactions entertained.

The above discussion provides a justification of GMA from a model robustness and efficiency point of view. Notice that $B_s(d)$ provides a kind of overall

measure of the partial aliasing and correlation among factorial effects, and so indirectly takes efficiencies into account. The conclusion we draw here is also supported by extensive empirical studies, some of which will be reported in the next section.

Remark 1. It can be seen that for orthogonal main-effect plans (e.g., those constructed from Hadamard matrices), if $f = 1$, then both $D_1(d)$ and $S_1^2(d)$ depend only on $B_3(d)$: $D_1(d) = 1 - 3B_3(d)/\binom{m}{2}$ and $S_1^2(d) = 6B_3(d)/\binom{m}{2}$. In this case, maximizing $D_1(d)$, minimizing $S_1^2(d)$ and minimizing $B_3(d)$ are all equivalent.

4. Empirical Study for 20-run Designs

We consider the ten designs of twenty runs and five factors found by Lin and Draper (1992) and further studied by Wang and Wu (1995). These designs are labeled as 5.1, 5.2, ..., 5.10 in Deng, Li and Tang (2000), with the meaning that design 5. i is the i th best among the ten designs according to GMA. Table 1 gives the D_f values for the ten designs, $f = 1, \dots, 10$. Consistency between the GMA ranking and the D_f ranking is evident.

Table 1. List of D_f for $1 \leq f \leq 10$.

design	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	D_9	D_{10}
5.1	0.8800	0.7573	0.6369	0.5233	0.4199	0.3293	0.2525	0.1894	0.1392	0.1002
5.2	0.8800	0.7589	0.6403	0.5277	0.4239	0.3311	0.2509	0.1838	0.1297	0.0880
5.3	0.8800	0.7391	0.5889	0.4416	0.3086	0.1984	0.1155	0.0597	0.0267	0.0099
5.4	0.8800	0.7418	0.5946	0.4486	0.3138	0.1992	0.1106	0.0502	0.0157	0.0000
5.5	0.7840	0.5952	0.4362	0.3075	0.2075	0.1333	0.0807	0.0453	0.0230	0.0099
5.6	0.7840	0.5956	0.4366	0.3069	0.2051	0.1284	0.0734	0.0363	0.0131	0.0000
5.7	0.7840	0.5770	0.3948	0.2480	0.1405	0.0699	0.0293	0.0096	0.0019	0.0000
5.8	0.6880	0.4535	0.2847	0.1687	0.0932	0.0471	0.0211	0.0078	0.0019	0.0000
5.9	0.6880	0.4353	0.2499	0.1273	0.0552	0.0187	0.0039	0.0000	0.0000	0.0000
5.10	0.6880	0.4358	0.2496	0.1257	0.0531	0.0171	0.0032	0.0000	0.0000	0.0000

Table 2 lists the values of $S_f^2(d)$ for the ten designs. By Proposition 1, we expect to see consistency between the GMA ranking and the S_f^2 ranking when f is relatively small. As it turns out, the S_f^2 ranking is the same as the GMA ranking for all $f \leq F (= 10)$. To quantify the degree of consistency between the D_f -criterion and the S_f^2 -criterion, we calculate the correlation coefficient $\rho(D_f, S_f^2)$ between D_f and S_f^2 . The values of $|\rho(D_f, S_f^2)|$ are given in Table 2. When $f \leq 6$, $|\rho(D_f, S_f^2)| \geq 0.95$. Of course, as mentioned in Remark 1, when $f = 1$, D_1 and S_1^2

are equivalent and $|\rho(D_1, S_1^2)| = 1$. The correlation (and hence the consistency) between D_f and S_f^2 is very high, especially when f is relatively small.

Table 2. List of S_f^2 and $|\rho(D_f, S_f^2)|$ for $1 \leq f \leq 10$.

design	S_1^2	S_2^2	S_3^2	S_4^2	S_5^2	S_6^2	S_7^2	S_8^2	S_9^2	S_{10}^2
5.1	0.24	0.51	0.80	1.12	1.47	1.84	2.24	2.67	3.12	3.60
5.2	0.24	0.51	0.80	1.12	1.47	1.84	2.24	2.67	3.12	3.60
5.3	0.24	0.55	0.93	1.38	1.89	2.48	3.14	3.86	4.65	5.52
5.4	0.24	0.55	0.93	1.38	1.89	2.48	3.14	3.86	4.65	5.52
5.5	0.43	0.89	1.38	1.89	2.43	2.99	3.58	4.20	4.85	5.52
5.6	0.43	0.89	1.38	1.89	2.43	2.99	3.58	4.20	4.85	5.52
5.7	0.43	0.93	1.50	2.14	2.85	3.63	4.48	5.40	6.38	7.44
5.8	0.62	1.27	1.95	2.66	3.39	4.14	4.93	5.74	6.57	7.44
5.9	0.62	1.32	2.08	2.91	3.81	4.79	5.82	6.93	8.11	9.36
5.10	0.62	1.32	2.08	2.91	3.81	4.79	5.82	6.93	8.11	9.36
$ \rho(D_f, S_f^2) $	1.0000	0.9993	0.9967	0.9908	0.9784	0.9544	0.9128	0.8526	0.7827	0.7198

Another important criterion to be considered is the estimation capacity defined in Cheng, Steinberg and Sun (1999). As mentioned in Section 3, the definition of estimation capacity can be carried over to nonregular designs without change: for any $1 \leq f \leq F$, $E_f(d)$ is the number of models with all the main effects and f two-factor interactions that can be estimated under d . In Table 3, we tabulate $\binom{F}{f} - E_f(d)$, the number of non-estimable models of the $\binom{F}{f}$ possible models.

Table 3. $\binom{F}{f} - E_f(d)$, number of non-estimable models with f two-factor interactions.

Design	$f \leq 3$	$f = 4$	$f = 5$	$f = 6$	$f = 7$	$f = 8$	$f = 9$	$f = 10$
5.1	0	0	0	0	0	0	0	0
5.2	0	0	0	0	0	0	0	0
5.3	0	0	0	0	0	0	0	0
5.4	0	0	0	1	4	6	4	1
5.5	0	0	0	0	0	0	0	0
5.6	0	0	0	0	1	3	3	1
5.7	0	0	0	0	0	1	2	1
5.8	0	0	0	0	0	1	2	1
5.9	0	4	24	58	72	45	10	1
5.10	0	5	30	73	84	45	10	1
$\binom{F}{f}$	—	210	252	210	120	45	10	1

While the GMA ranking is quite consistent with the rankings based on D_f and S_f^2 , the consistency between the GMA criterion and the estimation capacity criterion is only moderate. This may be because the estimation capacity criterion does not take efficiencies into consideration. Nevertheless, the top designs under the GMA criterion perform the best with respect to the estimation capacity criterion.

Appendix. Proof of Proposition 1.

We need to calculate the sum of squares of all the off-diagonal entries of $\mathbf{M}_{\mathcal{F}}(d)$. The blocks in the partitioned matrix (3.1) will be considered separately.

First of all, the f entries of $\mathbf{1}'_n \mathbf{Y}_{\mathcal{F}}(d)$ are the $j_S(d)$'s for $S \in \mathcal{F}$. Thus the sum of squares of all the entries of $\frac{1}{n} \mathbf{1}'_n \mathbf{Y}_{\mathcal{F}}(d)$ is equal to $\frac{1}{n^2} \sum_{S \in \mathcal{F}} [j_S(d)]^2$. Also, since each off-diagonal entry of $\mathbf{X}(d)' \mathbf{X}(d)$ is a $j_S(d)$ for some $S \in \mathcal{P}$, the sum of squares of all the off-diagonal entries of $\frac{1}{n} \mathbf{X}(d)' \mathbf{X}(d)$ is equal to $2 \frac{1}{n^2} \sum_{S \in \mathcal{P}} [j_S(d)]^2 = 2B_2(d)$.

Each entry of $\mathbf{X}(d)' \mathbf{Y}_{\mathcal{F}}(d)$ is $j_{i \Delta S}(d)$, for some $i \in \{1, \dots, m\}$ and $S \in \mathcal{F}$. Therefore the sum of squares of all the entries of $\frac{1}{n} \mathbf{X}(d)' \mathbf{Y}_{\mathcal{F}}(d)$ is equal to $\frac{1}{n^2} \sum_{i=1}^m \sum_{S \in \mathcal{F}} [j_{\{i\} \Delta S}(d)]^2$. Similarly, the sum of squares of all off-diagonal entries of $\frac{1}{n} \mathbf{Y}_{\mathcal{F}}(d)' \mathbf{Y}_{\mathcal{F}}(d)$ is $\frac{1}{n^2} \sum \sum_{S, T \in \mathcal{F}, S \neq T} [j_{S \Delta T}(d)]^2$. Therefore the sum of squares of all off-diagonal entries of $\mathbf{M}_{\mathcal{F}}(d)$ is

$$2B_2(d) + \frac{1}{n^2} \left\{ 2 \sum_{S \in \mathcal{F}} [j_S(d)]^2 + 2 \sum_{i=1}^m \sum_{S \in \mathcal{F}} [j_{\{i\} \Delta S}(d)]^2 + \sum_{S, T \in \mathcal{F}, S \neq T} [j_{S \Delta T}(d)]^2 \right\}. \tag{A.1}$$

By an elementary property of simple random sampling,

$$E_{\mathcal{F}} \left\{ \sum_{S \in \mathcal{F}} [j_S(d)]^2 \right\} = \frac{f}{F} \sum_{S \in \mathcal{P}} [j_S(d)]^2 = \frac{f}{F} n^2 B_2(d), \tag{A.2}$$

$$E_{\mathcal{F}} \left\{ \sum_{i=1}^m \sum_{S \in \mathcal{F}} [j_{\{i\} \Delta S}(d)]^2 \right\} = \frac{f}{F} \sum_{i=1}^m \sum_{S \in \mathcal{P}} [j_{\{i\} \Delta S}(d)]^2, \tag{A.3}$$

$$E_{\mathcal{F}} \left\{ \sum \sum_{S, T \in \mathcal{F}, S \neq T} [j_{S \Delta T}(d)]^2 \right\} = \frac{f(f-1)}{F(F-1)} \sum \sum_{S, T \in \mathcal{P}, S \neq T} [j_{S \Delta T}(d)]^2. \tag{A.4}$$

If $i \in \{j, k\}$, say $i = j$, then $\{i\} \Delta \{j, k\} = \{k\}$; in this case $j_{\{i\} \Delta \{j, k\}}(d)$ is zero. On the other hand, if $i \notin \{j, k\}$, then $\{i\} \Delta \{j, k\} = \{i, j, k\}$, and so $j_{\{i\} \Delta \{j, k\}}(d) = j_{\{i, j, k\}}(d)$. Counting all possible $\{i\}$'s and $\{j, k\}$'s, we see that $\sum_{i=1}^m \sum_{S \in \mathcal{P}} [j_{\{i\} \Delta S}(d)]^2 = 3n^2 B_3(d)$. Therefore by (A.3),

$$E_{\mathcal{F}} \left\{ \sum_{i=1}^m \sum_{S \in \mathcal{F}} [j_{\{i\} \Delta S}(d)]^2 \right\} = 3 \frac{f}{F} n^2 B_3(d). \tag{A.6}$$

Similarly, for $S = \{i, j\}$ and $T = \{k, l\}$, if S and T are disjoint, then $S \triangle T = \{i, j, k, l\}$; if S and T has exactly one element in common, say $i = k$, then $S \triangle T = \{j, l\}$. By simple counting, we have $\sum \sum_{S, T \in \mathcal{P}, S \neq T} [j_{S \triangle T}(d)]^2 = n^2 [6B_4(d) + 2(m-2)B_2(d)]$.

By (A.1), (A.2), (A.4) and (A.6),

$$S_f^2(d) = 2 \left[1 + \frac{f}{F} + \frac{f(f-1)}{F(F-1)}(m-2) \right] B_2(d) + 6 \frac{f}{F} B_3(d) + 6 \frac{f(f-1)}{F(F-1)} B_4(d).$$

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