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Efficient rounding of approximate designs

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SUMMARY

Discretization methods to round an approximate design into an exact design for a given sample size n are discussed. There is a unique method, called efficient rounding, which has the smallest loss of efficiency under a wide family of optimality criteria. The efficient rounding method is a multiplier method of apportionment which otherwise is known as the method of John Quincy Adams or the method of smallest divisors.

1. INTRODUCTION

In approximate design theory a design assigns to a number, say l, of points in some underlying design space weights $w_1, \ldots, w_l \in [0, 1]$ which sum to one, directing the experimenter to draw the fraction w_i of all observations under experimental condition i. For the design to become realizable for a fixed sample size n, the weights w_i must be discretized to integers n_i which sum to n. One approach is to calculate the quota nw_i, also called the fair share, and to rely on the usual numerical rounding of nw_i to the closest integer n_i. However, the numbers n_i so obtained need not sum to n.

As an example consider rounding the weights w_i to three digits, which is just another manifestation of the problem of discretizing the design weights for a sample of size $n = 1000$. The 20 A-optimal designs for polynomial regression listed by Pukelsheim & Torsney (1991, pp. 1622–3) may serve as an example. Only half of them sum to one, whereas the counts of the sets of weights which sum to 0·998, 0·999, 1·001, 1·002 are three, five, one, one, respectively. This is in line with the results of Mosteller, Youtz & Zahn (1967) and Diaconis & Freedman (1979) that the probability that rounded percentages not sum to one is clearly positive.

In the present paper we argue that there is another rounding procedure which performs much better. The literature contains some remarks that the asymptotic efficiency loss due to rounding stays bounded of order n^{-1}. In the case of differentiability the order improves to n^{-2}. In §§ 2 and 3 we use G- and D-optimal approximate and exact designs to illustrate that these orders are generally best possible. On the other hand these examples make it clear that the asymptotic results are misleading if anything, when it comes to finding apportionment methods which work well for any finite sample size n.

In § 4 we discuss the class of multiplier methods. Every discretization method in this class is sample size monotone, that is, if n increases then the discretizations n_i do not decrease. This is investigated in detail by Balinski & Young (1982) who study methods of apportionment for electorial bodies. The problem in political science contexts is that there is no clear-cut optimality criterion to justify a specific choice out of the ensemble of all multiplier methods.

In contrast experimental design theory provides a wide selection of optimality criteria, such as the D-, A-, E-criteria and others. In § 5 we deduce an efficiency bound which holds uniformly over the class of all such criteria that are of interest in experimental design. We then set out to optimize the efficiency bound. The best bound is attained for a unique multiplier method which is based on efficient rounding, otherwise known as the method of John Quincy Adams or method of smallest divisors (Balinski & Young, 1982). Of the various ways to characterize the efficient rounding procedure, one which is particularly rewarding from the statistical point of view is based on the likelihood ratios of the standardized discretizations n_i/n relative to the true weights w_i.

2. Asymptotic order $O(n^{-1})$

Kiefer (1959, p. 281; 1960, p. 383) mentions that given an approximate design with weights $w_1, \ldots, w_l$ there exists an exact design with frequencies $n_1, \ldots, n_l$ for sample size $n = \Sigma_{i \le l} n_i$ with criterion value to within order $O(n^{-1})$. To see that this order is generally best possible we need consider only linear regression with a single control variable in $[-1, 1]$ (Silvey, 1980, p. 4). In the approximate theory the G-optimal design assigns weights $\frac{1}{2}$ to the two endpoints ± 1. In the exact theory the G-optimal design assigns frequencies m to ± 1 if $n = 2m$ is even, while adding an additional observation at zero if $n = 2m + 1$ is odd. Straightforward evaluation of the G-criterion yields efficiency loss $1/(2n-1)$ or 0 for $n = 2m+1$ or $n = 2m$, respectively. Hence the order is $O(n^{-1})$.

In this example the exact G-optimal design calls for an additional support point at zero if n is odd. Furthermore the remarks of Gaffke & Krafft (1982, p. 397) suggest that for quadratic regression the exact G-optimal design has support points ± 1, $\pm\alpha(n)$, 0 of which $\alpha(n)$ varies with sample size n. This is just another illustration of the well-known fact that the problem of finding an exact optimal design is quite intricate. Bandemer & Näther (1980, § 4.4.5) present several round-off strategies which take into account the particulars of a given specific optimality criterion. However, we do not aim to solve an exact design problem. Rather we want to find a rounding method which works well uniformly over all reasonable criteria, and which is simple to handle. Therefore we restrict attention to those methods which maintain the l support points that belong to the given approximate design.

For instance, the approximate G-optimal design for linear regression with a single control variable has support points ± 1. If $n = 2m+1$ is odd then for the points ± 1 the frequencies $m+1$ and m, or m and $m+1$ are natural discretizations. Under the G-criterion either choice has efficiency loss equal to $1/n = O(n^{-1})$. Thus the restriction to the support points ± 1 increases the efficiency loss from $1/(2n-1)$ to $1/n$, but does not change the asymptotic order $O(n^{-1})$.

3. Asymptotic order $O(n^{-2})$

If the optimality criterion is differentiable at the optimal design weights then the gradient term in the Taylor expansion vanishes whence the efficiency loss becomes bounded of order n^{-2}. The subtleties are in the differentiability assumptions which permit an application of Taylor's theorem; see Pukelsheim (1992, Theorem 12.10) and unpublished reports by J. Fellman and S. Rieder. In the case of differentiability the order $O(n^{-2})$ is best possible, as is shown by the following example.

Consider a dth-degree polynomial regression with a single control variable over $[-1, 1]$. The approximate D-optimal design assigns uniform weight $1/k$ to each of $k = d+1$ support points (Silvey, 1980, p. 43). For the exact problem we represent the sample size $n = mk + r$ as an integer multiple m of k plus a remainder $r \in \{0, \ldots, k-1\}$. It seems natural to consider the discretizations which come as close as possible to the uniform weights $1/k$, that is, which assign frequency $m+1$ to r points and frequency m to the remaining $k-r$ points. A remarkable result of Gaffke (1987) says that these discretizations are exactly D-optimal, except for a few small values of n. In other words, these discretizations have the smallest D-efficiency loss, and any other discretization performs worse.

In this example it is fairly straightforward to determine the constant in the $O(n^{-2})$ term. To this end we scale the D-efficiency loss by n^2/k^2 and introduce

$$\lambda_D(n) = \frac{n^2}{k^2}\left[1 - \frac{\det^{1/k}\{M(n)\}}{\det^{1/k}\{M(\infty)\}}\right], \tag{1}$$

where $M(n)$ is the $k \times k$ information matrix of the standardized exact D-optimal design for sample size n, with weights $(m+1)/n$ and m/n, while $M(\infty)$ is the information matrix of the approximate D-optimal design, with weights $1/k$. Following Gaffke (1987) and Pukelsheim (1992), direct evaluation of the determinants yields

$$\lambda_D(n) = (m+\alpha)\left\{m + \alpha - m\left(1 + \frac{1}{m}\right)^{\alpha}\right\}, \tag{2}$$

with remainder $\alpha = r/k \in [0, 1]$. The biggest loss is incurred in the first interval where the discretization effect is felt most,

$$\lambda_D(n) \leq \max_{\alpha \in [0,1]} (1+\alpha)(1+\alpha-2^{\alpha}) < 0{\cdot}135.$$

For large periods m the bound 0·135 tightens to 0·125, see Fig. 1.

Unfortunately the uniformity of the D-optimal weights makes it impossible to appreciate different discretization methods. Every reasonable method will lead to the frequencies $m+1$ and m as given above.

Nor does the Taylor expansion provide the right clue to discriminate between different apportionment methods. The estimate of the remainder term is based on the principles

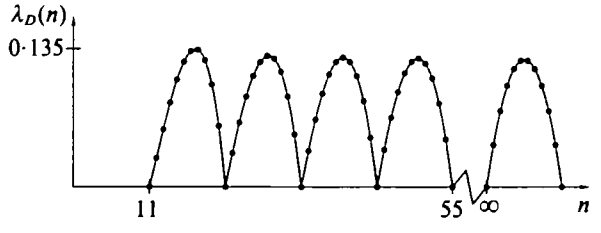

Fig. 1. Asymptotic efficiency loss of order $O(n^{-2})$. The dots indicate the scaled efficiency loss $\lambda_D(n)$ of (1) and (2), of the standardized exact D-optimal design for sample size n relative to the approximate D-optimal design, in a polynomial regression of degree $d = 10$ with a single control variable over $[-1, 1]$. The bound 0·135 does not depend on the degree d of the model, and asymptotically tightens to 0·125.

of calculus, not statistics. Kiefer (1971, p. 116) chooses to minimize the total variation distance $\max_{i \leq l} |n_i/n - w_i|$. The method of Hamilton is the unique apportionment method which minimizes this sup-norm or any other l_p-norm (Balinski & Young, 1982, p. 104). A systematic analysis shows that this method is seriously flawed, and Balinski & Young review the political complications that arose with its use in the history of the U.S.A. For design purposes it suffices to notice that the method of Hamilton is not sample size monotone. In other words, a sequential application of the rule may lead to the situation that for sample size $n+1$ the Hamilton apportionment calls for the removal of an observation which was part of the discretization of sample size n.

4. Multiplier methods

The defect of the method of Hamilton is that it is too concerned with the quotas nw_i. It ignores the problems that are caused by which procedure is used to round nw_i to n_i, and whether it applies to all quotas $nw_1, \ldots, nw_l$ equally fairly. Multiplier methods reverse the issue. Every multiplier method corresponds to a rounding procedure R. This is a monotone function rounding a real number z to one of the two integers closest to z or to both; see § 5. The rounding procedure R is then applied to the pseudoquotas $\nu w_1, \ldots, \nu w_l$, where $\nu \geqslant 0$ is some multiplier such that the rounded numbers $R(\nu w_i)$ sum to n. The point is that every pseudoquota νw_i gets rounded using the same method R. The multiplier ν has no meaning other than being a technical tool.

As the multiplier ν increases so do the frequencies $R(\nu w_i)$ and their sum $\Sigma_{i \leq l} R(\nu w_i)$. Hence for two sample sizes $\tilde{n} > n$ a multiplier $\tilde{\nu}$ which works for the large sample size $\tilde{n}$ cannot fall below a multiplier ν for the small sample size n. This proves that every multiplier method is sample size monotone.

There is another advantage of multiplier methods of apportionment. Due to limited machine precision the weights w_i often do not sum to one on a computer. This calls for the normalization w_i/μ, with $\mu = \Sigma_{i \leq l} w_i$. But a multiplier method yields the same result whether based on w_i, or on w_i/μ. In other words, multiplier methods are stable against numerical inaccuracies.

Thus our problem now reduces to finding a rounding procedure R which is appropriate for the design of experiments. Fedorov (1972, p. 157) argues that the discretizations n_i of the approximate weights w_i ought to fulfil

$$n_i \geqslant \lceil (n-l)w_i \rceil \quad (i = 1, \ldots, l). \tag{3}$$

Here the function $\lceil . \rceil$ means to round up to the next integer. Appendix B of Balinski & Young (1982) shows that of the five classical multiplier methods that are associated with the names of Adams, Dean, Hill, Webster and Jefferson only that of Adams respects the Federov minimum apportionment (3). We conjecture but are unable to prove that this extends to all multiplier methods. However, there is an alternative and more convincing approach which distinguishes the Adams method even among all apportionment methods, including those which are not multiplier methods.

To this end let ξ denote the approximate design which assigns weight w_i to the support point x_i, for $i = 1, \ldots, l$. For any other approximate design η we define the minimum likelihood ratio of η relative to ξ,

$$\varepsilon_{\eta/\xi} = \min_{i \leq l} \frac{\eta(x_i)}{w_i}. \tag{4}$$

Then we have

$$E_\eta(xx^T) \geq \sum_{i<l} \eta(x_i) x_i x_i^T \geq \varepsilon_{\eta/\xi} \sum_{i<l} w_i x_i x_i^T = \varepsilon_{\eta/\xi} E_\xi(xx^T).$$

That is, the information matrices of η and ξ (Silvey, 1980, p. 15) satisfy

$$M(\eta) \geq \varepsilon_{\eta/\xi} M(\xi). \tag{5}$$

Now we consider a specific optimality criterion ϕ, a real-valued function defined on the nonnegative definite $k \times k$ matrices, and assume that ϕ is matrix isotonic and positively homogeneous. This embraces virtually all of the classical criteria. For instance the D-, A- and E-criteria correspond to $\phi_D(M) = \det^{1/k} M$, $\phi_A(M) = (\operatorname{tr} M^{-1}/k)^{-1}$, and $\phi_E(M)$ equals the smallest eigenvalue of M. For any such ϕ, (5) entails

$$\phi(M(\eta)) \geq \phi(\varepsilon_{\eta/\xi} M(\xi)) = \varepsilon_{\eta/\xi} \phi(M(\xi)).$$

In other words, $\varepsilon_{\eta/\xi}$ from (4) provides a lower bound on the ϕ-efficiency ratio $\phi(M(\eta))/\phi(M(\xi))$. We call $\varepsilon_{\eta/\xi}$ the efficiency bound of η relative to ξ. It holds uniformly over all criteria ϕ which are matrix isotonic and positively homogeneous, and it applies to the information matrices (5).

For the discretization issue we consider a standardized exact design $\eta(x_i) = n_i/n$. We have now arrived at a specific optimization problem, to find a discretization n_i which has the best efficiency bound. That is, we wish to solve $\max_{n_1,\ldots,n_l} \min_{i<l} n_i/w_i$. The solution is the Adams apportionment, see Proposition 3.10 of Balinski & Young (1982, p. 105), or Pukelsheim (1992, Theorem 12.7). Thus the Adams apportionment is the most efficient discretization method for the design of experiments. In the next section we discuss the rounding procedure which underlies the Adams apportionment, and which we call efficient rounding.

5. Efficient rounding

The rounding procedure which underlies the Adams apportionment is the one where fractional numbers z always get rounded up to the next integer, while integers z may be rounded up or not. Because of the latter ambiguity the rounding $\lceil z \rceil$ is defined to be a one- or two-element set, rather than a number $R(z)$ as in § 4,

$$\lceil z \rceil = \begin{cases} \{k+1\} & \text{for } z \in (k, k+1), \\ \{k, k+1\} & \text{for } z = k, \end{cases}$$

for all integers k. The corresponding multiplier method results in a set of apportionments $E(\xi, \eta)$ which consists of those discretizations $(n_1, \ldots, n_l)$ such that the frequencies n_i lie in $\lceil \nu w_i \rceil$ and fulfil $\Sigma_{i<l} n_i = n$, for some multiplier $\nu \geq 0$. We call $\lceil . \rceil$ the efficient rounding procedure, and $E(\xi, n)$ the efficient design apportionment.

The fact that an efficient apportionment $E(\xi, n)$ may be a set rather than a singleton is illustrated by the D-optimal designs of § 3. For sample size $n = mk + r$ there are $k!/\{r!(k-r)!\}$ possible ways to assign the frequencies $m+1$ and m to the available support points. These assignments make up the set $E(\xi, n)$, and they appear equally persuasive. The reason is that the constant weights $w_i = 1/k$ do not provide enough information for the apportionment method to discriminate between these discretizations. The same phenomenon occurs when two or more weights are too close together rather than being exactly equal.

Under the efficient rounding a pseudoquota νw_i with a positive fraction is rounded up to the next integer regardless of how small the fraction is. Therefore if $n \geqslant l$ then every discretization in $E(\xi, n)$ has $n_i \geqslant 1$, and the support set stays the same as that of ξ. It follows that the associated information matrices have the same range, and provide the same set of identifiable parameter functions. One can also verify (Pukelsheim, 1992) that the efficiency bound $\varepsilon_{\eta/e}$ is the same whenever the standardized exact design $\eta(x_i) = n_i/n$ arises from some discretization $(n_1, \ldots, n_l)$ in $E(\xi, n)$, no matter which one. This shows that the efficiency bound is intrinsic to the set $E(\xi, n)$ rather than to any one of its members. Hence we define

$$\varepsilon_\xi(n) = \min_{i \leqslant l} \frac{n_i/n}{w_i},$$

with an arbitrary member $(n_1, \ldots, n_l)$ of $E(\xi, n)$. Having singled out the efficient rounding as the one which has the uniformly best efficiency bound we are left with the task of finding a quick way to calculate an appropriate multiplier ν.

6. Implementation

In our use of the efficient design apportionment we have found it fastest to proceed in two steps, to use the multiplier $\nu = n - l/2$ to apportion most of the observations, and to deal with the remaining observations individually. The multiplier $\nu = n - l/2$ is motivated as follows.

The multiplier $n - l$ of the Fedorov minimum apportionment (3) is generally too small since $n_i \in [\![(n-l)w_i]\!]$ implies

$$\textstyle\sum_{i \leqslant l} n_i \leqslant \sum_{i \leqslant l} \{(n-l)w_i + 1\} = n.$$

We tested this multiplier for the efficient apportionment of the E-optimal design for polynomial regression of degree 10, for $n = 11, \ldots, 1000$. The average discrepancy $(\Sigma_{i \leqslant l} n_i) - n$ turned out to be $-5{\cdot}499$. That is, on average the last $l/2 = 5{\cdot}5$ observations had to be assigned individually. On the other hand the multiplier n tends to be too large since $n_i \in [\![nw_i]\!]$ implies $\Sigma_{i \leqslant l} n_i \geqslant \Sigma_{i \leqslant l} nw_i = n$. As a compromise between $n - l$ and n we recommend the use of $\nu = n - l/2$.

For the 20 designs of Pukelsheim & Torsney (1991) the multiplier $n - l/2$ for $n = 1000$ yields the following discrepancy counts,

$(\sum_{i \leqslant l} n_i) - n$	-2	-1	0	1	2
counts	3	2	12	2	1

That is, in 60% of cases the multiplier $n - l/2$ gave the efficient design apportionment, while in 25% and 15% it assigns too few and too many observations, respectively.

This leads to problems of the following type. Given $(n_1, \ldots, n_l) \in E(\xi, n)$, where does the next observation go or which observation should be deleted to obtain an efficient apportionment of sample size $n+1$ or $n-1$? The optimality property of § 4, that the efficient apportionment maximizes $\min_{i \leqslant l} n_i/w_i$, provides the answer. For a transition from n to $n+1$, a frequency n_j such that n_j/w_j attains $\min_{i \leqslant l} n_i/w_i$ ought to be augmented to $n_j + 1$. Similarly, for a transition from n to $n-1$, a frequency n_k for which n_k/w_k attains $\max_{i \leqslant l} (n_i - 1)/w_i$ ought to be reduced to $n_k - 1$; compare Balinski & Young (1982, p. 100).

7. Efficiencies

Since the efficient design apportionment has an efficiency bound which is optimal it is not surprising that it obeys the asymptotic orders of §§ 2 and 3. If ξ is ϕ-optimal and differentiability holds then the order $O(n^{-2})$ applies, with a constant depending on ϕ and ξ. In contrast, order $O(n^{-1})$ is achieved by the efficiency bound itself irrespective of the criterion ϕ,

$$1 - \varepsilon_\xi(n) \leqslant l/n.$$

This estimate holds, not just asymptotically, but for every n. The bound l/n also applies to the loss of ϕ-efficiency, uniformly over all optimality criteria ϕ which are matrix isotonic and positively homogeneous. The constant l may be improved if a particular criterion ϕ is under study. For instance in the example of § 2 the G-efficiency loss is $1/n$, while the present bound is $2/n$.

For the 20 designs of Pukelsheim & Torsney (1991) we obtained the following results. In the ten cases where the numerical rounding fails to sum to one, the A-efficiency of the numerical rounding relative to the efficient rounding is clearly governed by the discrepancy of the numerical rounding and equals 0·998, 0·999, 1·001, 1·002 in the three, five, one, and one cases mentioned in § 1. Of the ten cases where the numerical rounding sums to one only six are rounded efficiently. For the other four the efficient rounding is different, and improves the A-criterion in one case while being the same up to order 10^{-5} in three cases. Of course, there is no guarantee that a particular criterion ϕ improves under the efficient rounding although our derivation suggests that this is more likely to happen than not.

The efficient apportionment results in a unique discretization in 16 out of the 20 cases. In the remaining four cases the efficient apportionment contains two discretizations which break the symmetry. For instance, the A-optimal design for degree six has efficient apportionment (65, 147, 185, 205, 185, 148, 65), or (65, 148, 185, 205, 185, 147, 65). In all four cases the A-criterion is constant. Another example where a transition to exact designs entails a loss of symmetry is given by Kiefer (1959, p. 281; 1971, p. 117).

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