The Annals of Statistics
1997, Vol. 25, No. 6, 2313–2327

LATTICE-BASED *D*-OPTIMUM DESIGN FOR FOURIER REGRESSION

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A theory of optimum orthogonal fractions is developed for Fourier regression models using integer lattice designs. These provide alternatives to simple grids (product designs) in the case when specified main effects and interaction terms are required to be analyzed. The challenge is to obtain sample sizes which are polynomial in the dimension rather than exponential. This is achieved for certain models with special algorithms based on both algebraic generation and more direct sequential search.

1. Introduction and preliminaries. Bates, Buck, Riccomagno and Wynn (1996) mention that integer lattice designs are *D*-optimum in the sense of Kiefer and Wolfowitz (1959) for Fourier regression models. It has been known for some years that equally spaced grids (product designs) have this property. In analogy to the situation of polynomial regression, we can reduce the size of the experiment by using a fraction if no or only a limited number of interactions are required to be estimated. Here the lattice will play the role of fractions in the polynomial theory. The alias structure turns out to be radically different with the cyclic group playing an important role via the harmonic nature of the theory. The lattice structure allows us to map a high-dimensional model into a suitable one-dimensional model.

For the one-dimensional Fourier regression model of order m,

$$E(Y(x)) = \theta_0 + \sqrt{2}\sum_{r=1}^{m}\sin(2\pi r x)\theta_r + \sqrt{2}\sum_{r=1}^{m}\cos(2\pi r x)\phi_r, \tag{1}$$

$x \in [0, 1)$, the equally spaced design points on an equidistant grid with, at least, $2m+1$ support points is *D*-optimum in the sense of Kiefer and Wolfowitz [see Hoel (1965)].

Note that these designs are optimum irrespectively of whether the normalizing factor $\sqrt{2}$ is included in the model equation (1) or not. A uniform design with exactly $2m + 1$ support points has minimal support; that is, there are exactly as many design points as there are parameters in the model.

Let $A_l = \{\alpha \in \{-1, 1\}^l;\ \alpha_1 = 1\}$ be the set of all l-dimensional multiindices from $\{-1, 1\}$ with unit first entry. Then a complete M-factor interaction model

Received June 1995; revised November 1996.

[1]Work supported by the UK Engineering and Physical Science Research Council.

[2]Work supported by Grants Ku719/2-1 and Ku719/2-2 of the Deutsche Forschungsgemeinschaft.

AMS 1991 *subject classifications*. 62K05, 62J99.

Key words and phrases. Fourier models, lattices, orthogonal fractions complexity.

can be written as follows:

$$
\begin{aligned}
&E(Y(x_1,\ldots,x_d))\\
&\quad=\theta_0+\sqrt{2}\sum_{l=1}^{M}\sum_{k_1<\cdots<k_l}\sum_{r_1=1}^{m_{k_1}}\cdots\sum_{r_l=1}^{m_{k_l}}\sum_{\alpha\in A_l}\sin(2\pi(\alpha_1 r_1 x_{k_1}+\cdots+\alpha_l r_l x_{k_l}))\\
&\qquad\qquad\times\theta_{k_1,\ldots,k_l,\,r_1,\ldots,r_l,\,\alpha}\qquad(2)\\
&\quad+\sqrt{2}\sum_{l=1}^{M}\sum_{k_1<\cdots<k_l}\sum_{r_1=1}^{m_{k_1}}\cdots\sum_{r_l=1}^{m_{k_l}}\sum_{\alpha\in A_l}\cos(2\pi(\alpha_1 r_1 x_{k_1}+\cdots+\alpha_l r_l x_{k_l}))\\
&\qquad\qquad\times\phi_{k_1,\ldots,k_l,r_1,\ldots,r_l,\alpha}
\end{aligned}
$$

$x=(x_1,\ldots,x_d)\in[0,1)^d$.

We introduce the notation $F(d;m_1,\ldots,m_d;M)$ for the complete Fourier model (2) in d dimensions with one-dimensional "marginal" models for $x_1,\ldots,x_d$ respectively of orders m_1 to m_d and in which all interactions up to M factors are included. In the present paper we place special emphasis on the particular cases of additive models $F(d;m_1,\ldots,m_d;1)$ without interactions and first order interaction models $F(d;m_1,\ldots,m_d;2)$, that is, on models with complete two-factor interactions.

Note that the general model (2) is equivalent to the complete M-factor interaction model

$$
E(Y(x_1,\ldots,x_d))=\theta_0+\sum_{l=1}^{M}\sum_{k_1<\cdots<k_l}(f_{k_1}(x_{k_1})\otimes\cdots\otimes f_{k_l}(x_{k_l}))^{\top}\beta_{k_1,\ldots,k_l},\qquad(3)
$$

with marginals $E(Y_k(x_k))=\theta_0+f_k(x_k)^{\top}\beta_k$ which has been investigated, for example, by Schwabe (1996a), in general. Here we consider the marginals $f_k(x_k)=\sqrt{2}(\sin(2\pi r x_k),\cos(2\pi r x_k))_{r=1,\ldots,m_k}^{\top}$. From the standard formulas for trigonometric functions of sums, it is seen that both models are linked by an orthogonal transformation matrix which does not affect the optimality criteria under consideration.

Hoel (1965) showed that *product designs* are D-optimum for Kronecker product–type models ($M=d$). Thus, if ξ_1 is a D-optimum design measure for a linear model $E(Y_1(x_1))=\sum_{i=0}^{m_1}\theta_i f_i(x_1)$ on a design space X_1 and if ξ_2 is D-optimum for a model $E(Y_2(x_2))=\sum_{i=0}^{m_2}\phi_i g_i(x_2)$ on a space X_2, then the product $\xi_1\times\xi_2$ (in the measure-theoretic sense) is D-optimum for the linear model $E(Y(x_1,x_2))=\sum_{i=0}^{m_1}\sum_{j=0}^{m_2}\beta_{ij}f_i(x_1)g_j(x_2)$ which includes all terms of the form $f_i(x_1)g_j(x_2)$ on the space $X_1\times X_2$. The same is true for additive models without interactions if $f_0=1$ and $g_0=1$ [see Schwabe (1996a)]. In general, the product $\xi_1\times\cdots\times\xi_d$ of marginally D-optimum designs ξ_k is D-optimum if a constant term is included in each marginal model [see Schwabe (1996a), Section 6.1]. For the case of Fourier regression, this last restriction is not necessary [see Schwabe (1996b)]. In additive models the optimality of product designs has been proved by Rafajłowicz and Myszka (1992) and by Schwabe

(1996a) for other criteria, including A-, E- and integrated mean squared error optimality.

If we use D-optimum designs with minimal support in the marginal Fourier models of order m_k, the number of support points for the product design is $\prod_{k=1}^{d}(2m_k+1)$ which coincides with the number of parameters in the Kronecker product–type complete interaction model ($M = d$). In general, this number is much larger than the number of parameters in a d-dimensional model. For example, if the orders of the marginal models coincide ($m_1 = \cdots = m_d = m$), then there are $dm+1$ parameters in the additive model $F(d; m, \ldots, m; 1)$ and $O(d^2)$ parameters in the two-factor interactions models. It is challenging, then, to obtain D-optimum design sequences for which the sample size does not increase much faster in the dimension d than the number of parameters. In particular, we will look for sequences of D-optimum designs with a polynomially increasing support rather than the exponentially increasing product designs.

The main purpose of the present paper is to show that optimality can be achieved by using lattice designs for complete Fourier models instead of product designs. Like the Fourier models themselves, such designs have a structure which is cyclic, but for which the aliasing theory is rather different from that for classical polynomial models. We shall give examples of optimum families of designs for specified complete Fourier models.

We consider lattices generated by a single-integer generator which therefore can be identified as one-dimensional objects. Let $g = (g_1, \ldots, g_d)$ be a d-dimensional vector with positive integer components and n a positive integer. The vector generates a finite number of line segments in the d-dimensional hypercube $[0,1)^d$; that is, the set $\{(tg_1 \bmod 1, \ldots, tg_d \bmod 1);\ t \in \mathbb{R}\}$ consists of a finite number of line segments intersecting $[0,1)^d$. If we identify the hypercube with the corresponding torus by matching opposite faces, then these line segments form a single closed line wrapped around the torus. The generated designs will be supported on these line segments and will be referred to as lattice designs.

The n-point lattice design generated by $(g_1, \ldots, g_d)$ is the uniform design supported on the grid

$$\left(\frac{j}{n}g_1 \bmod 1, \ldots, \frac{j}{n}g_d \bmod 1\right) = \left(\frac{jg_1 \bmod n}{n}, \ldots, \frac{jg_d \bmod n}{n}\right), \qquad j = 0, \ldots, n-1.$$

If g_1 and n are mutually prime, we may assume without loss of generality that $g_1 = 1$ [see Niederreiter (1992)]. This relabeling is achieved by a rearrangement of the design points. Note that the one-dimensional uniform design supported on n equally spaced points is a particular case of a lattice design generated by $g = (1)$.

2. Main statements. In this section we show how the generator $g = (g_1, \ldots, g_d)$ can be chosen for a given model $F(d; m_1, \ldots, m_d; M)$ such that

the n-point lattice design is D-optimum. In Section 2.1 we start with an illustrative example. In Section 2.2 the theoretical background is developed and conditions are elaborated which must be satisfied by g and n. Finally, in Section 2.3 an algorithm is presented to find families of D-optimum lattice designs for which the size increases polynomially in the dimension. Section 3 collects various applications to additive models and to two-factor interaction models. In the latter D-optimum designs are investigated for either the main effects only or for the whole parameter vector. Sequences of generators and alternative algebraic methods are determined by the algorithm of Section 2.3.

2.1. *Motivation.* A key observation in this paper is that a model with terms in higher dimensions can be mapped into a model in one dimension by exploiting the structure of the lattice. We start with the most simple two-dimensional example of the model $F(2;1,1;1)$ which has five parameters and we use the n-point lattice with generator $g = (1,3)$ and $n = 5$ support points.

For the model $F(2;1,1;1)$ the model equation (2) reduces to

$$E(Y(x_1(t), x_2(t))) = \theta_0 + \sqrt{2}\sin(2\pi t)\theta_1 + \sqrt{2}\cos(2\pi t)\phi_1 + \sqrt{2}\sin(2\pi 3t)\theta_2 + \sqrt{2}\cos(2\pi 3t)\phi_2$$

on the line segments $(tg_1 \bmod 1, tg_2 \bmod 1) = (t, 3t \bmod 1)$ by the periodicity of the trigonometric functions. Hence, the model can be identified with a one-dimensional incomplete Fourier model in the variable t. Moreover, the five-point lattice design generated by $g = (1,3)$ is an equally spaced design with five support points on the line segments considered as a line on the torus.

The information matrices coincide in both the original two-dimensional model $F(2;1,1;1)$ and in the derived one-dimensional model on the line segments. Now, it can be checked that the five-point equally spaced design is D-optimum for the derived one-dimensional model (see Lemma 1). Hence, the information matrix is a multiple of the identity which, in turn, proves the D-optimality of the five-point lattice design for the original model. Note that the product design requires nine design points.

2.2. *General results.* We start by formulating in our terminology the Hoel (1965) result on the optimality of equidistant designs for one-dimensional Fourier models.

THEOREM 1. *For the one-dimensional model $F(1;m;1)$ the n-point lattice design generated by the integer g, $n \geq 2m+1$, is D-optimum if and only if, within the cyclic group $\mathscr{G}_n = (\{0,1,\ldots,n-1\},+)$, the cardinality of $\{0\} \cup g\mathscr{N}$ is $2m+1$ where $\mathscr{N} = \{r;\ r = -m,\ldots,-1,1,\ldots,m\}$.*

In other words, the n-point lattice design is D-optimum if and only if all members in $\mathscr{N}$ are distinct and different from 0 $(\bmod n)$. Note that the condition in Theorem 1 is satisfied if and only if all the parameters of the model are estimable; that is, D-optimality coincides with estimability for one-

dimensional lattice designs. We will see later on that this is also true for higher dimensions.

When all the entries in the array $\{0, rg;\ r \in \mathcal{N}\}$ are distinct in the set $\mathbb{Z}$ of all integers, they are also distinct in the cyclic group $\mathcal{G}_n$ if n is sufficiently large ($n \geq 2mg + 1$). Hence, $2mg + 1$ is an upper bound for the minimum sample size required, whereas a lower bound is given by the number of parameters in the model. Similar bounds are valid in higher dimensions.

The next result is a generalization of Theorem 1 and is helpful in proving the *D*-optimality of lattice designs.

LEMMA 1. *For the incomplete one-dimensional Fourier model,*

$$E(Y(x)) = \theta_0 + \sqrt{2}\sum_{j=1}^{q} \sin(2\pi r_j x)\theta_j + \sqrt{2}\sum_{j=1}^{q} \cos(2\pi r_j x)\phi_j, \tag{4}$$

where the r_j are distinct positive integers and the n-point lattice design generated by g is D-optimum for the subsystem $(\theta_0, \theta_1, \phi_1, \ldots, \theta_p, \phi_p)$ of parameters, $p \leq q$, if and only if, within the cyclic group $\mathcal{G}_n = (\{0, 1, \ldots, n-1\}, +)$,

(i) *the cardinality of the set $\{0\} \cup g\mathcal{N}'$ is $2p + 1$, where $\mathcal{N}' = \{\pm r_j;\ j = 1, \ldots, p\}$, and*

(ii) *$r_j \notin \{0\} \cup g\mathcal{N}'$ for $j = p + 1, \ldots, q$.*

PROOF. It is a fundamental property of trigonometric functions that

$$\sum_{j=0}^{n-1} \sin(2\pi(r+s)j/n) = \sum_{j=0}^{n-1} \cos(2\pi(r+s)j/n) = 0$$

if, and only if, $r \neq -s \bmod n$. With the standard formulas on trigonometric functions of sums, this yields

$$\begin{aligned}\sum_{j=0}^{n-1} \sin(2\pi rj/n)\sin(2\pi sj/n) &= \sum_{j=0}^{n-1} \sin(2\pi rj/n)\cos(2\pi sj/n) \\ &= \sum_{j=0}^{n-1} \cos(2\pi rj/n)\cos(2\pi sj/n) = 0\end{aligned}$$

if both $r \neq s \bmod n$ and $r \neq -s \bmod n$.

Hence, for a design satisfying (i) and (ii), the information matrix is block diagonal, and the relevant block associated with the parameters of interest equals n times the identity. This block can be identified as the information matrix of a *D*-optimum design for the submodel in which only the subsystem $(\theta_0, \theta_1, \phi_1, \ldots, \theta_p, \phi_p)$ of parameters is involved. Thus, by a simple refinement argument, the design is also *D*-optimum for the subsystem in the full model.

The converse can be checked by noticing that for $r = s \bmod n$ or $r = -s \bmod n$ the corresponding rows of the information matrix are linearly dependent and, hence, the parameters cannot be identified. □

The following theorem follows directly from Lemma 1 by embedding the model in the lattice and taking advantage of the one-dimensional structure so obtained.

THEOREM 2. *In the M-factor interaction model $F(d; m_1, \ldots, m_d; M)$, the n-point lattice design generated by $(g_1, \ldots, g_d)$ is D-optimum for the parameters up to the S-factor interactions $(S \leq M)$ if and only if the members in the first $S+1$ rows of the array*

$$
\begin{array}{lll}
0, & & \\
r_k g_k, & r_k \in \mathscr{N}_k, & k = 1, \ldots, d, \\
r_k g_k + r_l g_l, & r_k \in \mathscr{N}_k \text{ and } r_l \in \mathscr{N}_l, & 1 \leq k < l \leq d, \\
\vdots & & \\
r_{k_1} g_{k_1} + \cdots + r_{k_m} g_{k_m}, & r_{k_1} \in \mathscr{N}_{k_1}, \ldots, r_{k_m} \in \mathscr{N}_{k_m}, & 1 \leq k_1 < \cdots < k_m \leq d, \\
\vdots & & \\
r_{k_1} g_{k_1} + \cdots + r_{k_M} g_{k_M}, & r_{k_1} \in \mathscr{N}_{k_1}, \ldots, r_{k_M} \in \mathscr{N}_{k_M}, & 1 \leq k_1 < \cdots < k_M \leq d,
\end{array}
$$

where $\mathscr{N}_k = \{-m_k, \ldots, -1, 1, \ldots, m_k\}$, are distinct (in the cyclic group $\mathscr{G}_n$) and if they are, additionally (for $S < M$), different from those members in the last $M - S$ rows in $\mathscr{G}_n$.

The methodology of this paper consists of checking the entries in the various rows of the array in Theorem 2. For example, for the additive model $F(d; m_1, \ldots, m_d; 1)$, we check the first two rows. In some examples we shall seek to be able to estimate the main effects in the presence of possible interactions. For $M = 2$ it is necessary that the first two rows of the array are distinct and, in addition, the entries of the third row are distinct from the previous two. Strictly speaking, this yields D_s-optimality in the sense of Kiefer and Wolfowitz (1959) for the subset of main effect parameters. There is no difficulty in extending the orthogonality results in this way.

We have obtained the results in Section 3 as follows. First, we start from a generator and check whether all the members in the array of Theorem 2 are distinct in the set of all positive integers. If this is true, then they are also distinct in the cyclic group $\mathscr{G}_n$ with $n = 2n_{\max} + 1$, where $n_{\max}$ is the largest member in the array. We call this the *upper law*.

After that we look for smaller sizes n, maybe even minimal, such that the members remain distinct within the corresponding cyclic group $\mathscr{G}_n$. For example, a closer investigation of the array being considered for additive models shows that there are large gaps already at the beginning. To reduce the size, we can match the larger members of the array into suitable gaps left by the negative (in $\mathbb{Z}$) members which are concentrated in the upper half. Because of the symmetry of the array with respect to zero, the corresponding negative members will automatically fit into gaps left by the positive (in $\mathbb{Z}$) members in the lower half. Usually the largest gap will be between the maximum member

$n_{\max}$ and the next to maximum, say n_2, and in general $n_{\max} > n_2 + 1$. So a size $n_{\max} + n_2 + 1$ is suitable and gives a reduction of, at most, g_d. A similar rule holds for the other models. We call this the *generalized upper law*.

If we are interested only in the main effects, we may proceed as follows. If n_3 is the largest member in the first two rows of the array associated with the main effects and $n_{\max}$ is the largest member in the whole array described in Theorem 2, the *generalized upper law for main effects* states that a size $n_{\max} + n_3 + 1$ is suitable. Obviously, any size larger than the one given by the upper law or the generalized upper law for main effects is suitable.

REMARK. We note that due to invariance considerations [see Kiefer and Wolfowitz (1959) and Pukelsheim (1993), Chapter 13] the D-optimum designs obtained are also optimum with respect to any (convex) criterion based on the eigenvalues of the information matrix, including A- and E-optimality. This is true for the whole parameter vector as well as for the subsystems of the parameters up to the S-factor interactions (D_s-optimality). Moreover, those designs which are D-optimum for the whole parameter vector result in a minimum value for the integrated mean squared error

$$\int_0^1 \cdots \int_0^1 (\hat{Y}(x_1, \ldots, x_d) - E(Y(x_1, \ldots, x_d)))^2 \, dx_d \cdots dx_1,$$

where $\hat{Y}$ is the best linear unbiased predictor.

2.3. *An algorithm for the one-step strategy.* For every Fourier model the entries $g_1, \ldots, g_d$ of a generator $(g_1, \ldots, g_d)$ have to be different. Without loss of generality, we can look for generators with $1 = g_1 < \cdots < g_d$.

We present an algorithm for an iterative sequence of generator components obtained from Theorem 2 by a one-step strategy. A global search for the minimum g_d is possible, but we shall see that computer results for this simple strategy are in some agreement with theoretical procedures. Also, this algorithm gives a reasonable bound on the increase of the generator components and, hence, of the required size by the *upper law* as the dimension d increases.

For the generator $(g_1, \ldots, g_d)$ denote by $\mathscr{A}_d^{(M)}$ the set of all members in the array associated with a d-factor model with M-factor interactions. Further assume that we are interested in all the parameters up to the S-factor interactions, $1 \le S \le M$, and that the generator $(g_1, \ldots, g_d)$ is suitable. That is to say, the members in the first $S + 1$ rows of the array (including the first row containing only 0) are all distinct, and the members in the remaining last $M - S$ rows are distinct from those in the first $S + 1$ rows, but not necessarily different from each other (within the set $\mathbb{Z}$ of all integers). Then $\mathscr{A}_d^{(S)}$ is the set that collects the members of the first $S + 1$ rows of the array and, in particular, $\mathscr{A}_d^{(0)} = \{0\}$.

The following algorithm produces a sequence of generator components

Step 1. Start with $d = 1$ and $g_1 = 1$. Then (g_1) is suitable and $\mathscr{A}_1^{(S)} = \{-m_1, \ldots, -1, 0, 1, \ldots, m_1\}$, $1 \le S \le M$.

Step 2. If the generator $(g_1, \ldots, g_d)$ is suitable, then determine the set $\mathscr{A}_d^+ = \mathscr{A}_d^{(M)} + \mathscr{A}_d^{(S-1)}$ containing all sums of members of $\mathscr{A}_d^{(M)}$ and of its first S rows, respectively. Then add all integers for which any multiple up to order $2m_{d+1}$ is included in $\mathscr{A}_d^+$, that is, $\mathscr{A}_d^{++} = \bigcup_{r=1}^{2m_{d+1}} (1/r)\mathscr{A}_d^+ \cap \mathbb{Z}$.

Step 3. Let g_{d+1} be a positive integer not included in $\mathscr{A}_d^{++}$. Then the generator $(g_1, \ldots, g_d, g_{d+1})$ is suitable and $\mathscr{A}_{d+1}^{(S)} = \mathscr{A}_d^{(S)} \cup \bigcup_{r \in \mathscr{N}_{d+1}} \{r g_{d+1} + \mathscr{A}_d^{(S-1)}\}$ for $S = 1, \ldots, M$.

Step 4. Set $d := d + 1$ and go to Step 2.

For $S = 1$ we are only interested in the main effects. For $S = 2$ we are interested in the main effects and, additionally, all two-factor interactions. Finally, for $S = M - 1$ we are interested in all but the M-factor interactions and for $S = M$ we are interested in all parameters.

In the particular situation of equal order of Fourier regression in all factors, the constructions in the algorithm guarantee that $g_d = O(d^{M+S-1})$, as $d \to \infty$, because the cardinality of $\mathscr{A}_d^{(S)}$ increases like $O(d^S)$ and hence the cardinality of $\mathscr{A}_d^{++}$ increases, at most, as $O(d^{M+S-1})$. Consequently, if g_{d+1} is chosen as the smallest positive integer not belonging to $\mathscr{A}_d^{++}$, the iterative sequence of generator components and the corresponding sizes increase polynomially. This is to be compared to exponential growth for generators of the form $(1, a, a^2, \ldots, a^{d-1})$ (*power generators*) and generators defined by linear recursions (*Fibonacci-type* generators). Note that the total number of parameters increases polynomially like d^M and the number of parameters of interest increases like d^S.

3. Examples and constructions. The design generated by the power generator

$$(g_1, \ldots, g_d) = \left(1, 2m_1 + 1, (2m_1 + 1)(2m_2 + 1), \ldots, \prod_{k=1}^{d-1} (2m_k + 1)\right),$$

with $\prod_{k=1}^{d} (2m_k + 1)$ supporting points is optimum for all M-factor interaction models $F(d; m_1, \ldots, m_d; M)$, $1 \le M \le d$. However, the number of design points is, in general, much larger than the number of parameters, only being the same in the case $M = d$.

3.1. *Additive model.* For additive models we have only to check the first two rows of the array given in Theorem 2.

3.1.1. *Power-type generators.* In the additive Fourier model $F(d; m, \ldots, m; 1)$ with equal orders of the Fourier regressions in each component, the upper law gives a sample size of $n = 2m(2m + 1)^{d-1} + 1$ for the preceding power generator which increases exponentially in the dimension while the number of parameters is linear in d. While noticing that there is an unnecessary gap in the array between m and $2m + 1$, we obtain the power generator

$$(g_1, \ldots, g_d) = (1, m + 1, (m + 1)^2, \ldots, (m + 1)^{d-1}),$$

with minimum base $m+1$ for which the upper law gives an exponentially increasing size $n = 2m(m+1)^{d-1}+1$.

More generally, for $F(d; m_1, \ldots, m_d; 1)$ we can use the *generalized power generator*

$$(g_1, \ldots, g_d) = \left(1, m_1+1, (m_1+1)(m_2+1), \ldots, \prod_{k=1}^{d-1}(m_k+1)\right)$$

with size $n = 2m_d \prod_{k=1}^{d-1}(m_k+1)+1$.

3.1.2. *Recursively defined generators.* From Theorem 2 we see that a $(d-1)$-dimensional generator $(g_1, \ldots, g_{d-1})$ is suitable if and only if 0 and all $r_k g_k$, $r_k \in \mathcal{N}_k$, $k = 1, \ldots, d-1$, are distinct in $\mathbb{Z}$.

If we choose the next component g_d greater than the largest member of the preceding set, then the resulting generator $(g_1, \ldots, g_d)$ produces an array in which again all members are distinct. At each step the largest member will be $m_d g_d$. As it is reasonable to choose g_d as small as possible in order to reduce the gaps, we obtain the following linear recursion formula:

$$g_d = m_{d-1} g_{d-1} + 1,$$

with an initial value $g_1 = 1$ as usual. According to the upper law, the corresponding size is $n = 2m_d g_d + 1$. In particular, for the additive models $F(d; m, \ldots, m; 1)$ with equal orders in the components, we get $g_d = (m^d - 1)/(m-1)$ and a size $n = (2m^{d+1} - m - 1)/(m-1)$ in case $m \geq 2$. This size is smaller than the size of the power generator designs, but it is still exponentially increasing. For $m = 1$ the generator sequence simplifies to $g_d = d$ which increases linearly and the corresponding design has minimal support $(n = 2d+1)$.

3.1.3. *One-step generators and linear generators.* For the model $F(d; 1, \ldots, 1; 1)$ the one-step strategy obviously produces the same sequence $g_d = d$ of generator components as the recursive scheme given previously which is optimum in the sense that a minimal size n can be achieved which is equal to the number of parameters.

For the model $F(d; 2, \ldots, 2; 1)$ the algorithm of Section 2.3 produces the generator sequence

$$(1, 3, 4, 5, 7, 9, 11, 12, 13, 15, 16, 17, 19, 20, 21, 23, 25, 27, 28, 29, \ldots),$$

with corresponding minimal sizes

$$10, 13, 17, 23, 29, 34, 37, 41, 47, 49, 53, 59, 61, 65, 71, 77, 83, 87, 89, \ldots$$

for $d \geq 2$ which was found by exhaustive search. We notice that all odd numbers are included in the sequence of generator components. Hence, $g_d \leq 2d-1$ and the corresponding size increases linearly in the dimension d. The last observation suggests a simple alternative sequence of generator components

$$g_d = 2d - 1.$$

It can be proved that these linearly generated designs are suitable and that the minimum obtainable size is $n = 4d + 2$. Note that this size is, in fact, smaller than the size obtained for the one-step strategy if $d = 5, 6, 7, \ldots$.

The construction of such *linear generators* can be extended directly to the additive model $F(d; m, \ldots, m; 1)$ of general order m by

$$g_d = (d-1)m + 1$$

and the size $n = 2(d-1)m^2 + 2m + 1$ obtained by the upper law increases linearly in d. For the additive model $F(d; 3, \ldots, 3; 1)$ with third-order Fourier regression, the sequence $g_d = 3d - 2$ produces minimum obtainable sizes of $n = 17$ for $d = 2$ and $n = 9d$ for $d \geq 3$.

In the general case of unequal orders m_k, we use the generating procedure $g_k = (k-1)m + 1$ where $m = \max_k m_k$. The model is a submodel of $F(d; m, \ldots, m; 1)$. Hence, the entries in the corresponding array are distinct and the generated design is D-optimum if n is sufficiently large ($n \geq 2\max_k\{m_k g_k\} + 1$).

3.2. *Models with two-factor interactions.* For the complete two-factor interaction model $F(d; m_1, \ldots, m_d; 2)$, we have to check the first three lines of the array given in Theorem 2.

The power generator introduced in the beginning of Section 3 produces a sample size which is slightly smaller than the size for a product-type design. In the following we consider models $F(d; m, \ldots, m; 2)$ with equal orders in the components and we will be interested in either the main effects ($S = 1$) or the whole parameter vector ($S = 2$). We compare the performances of the minimum power generator, the recursively defined generators and the one-step generator.

3.2.1. *The model* $F(d; 1, \ldots, 1; 2)$. First, we study inference on the parameters associated with the main effects. The minimum power generator is $(1, 3, \ldots, 3^{d-1})$ and the size increases exponentially with base 3. An iterative sequence of generator components is given by the recursion formula $g_d = 2g_{d-1} + 1$. Hence, $g_d = 2^d - 1$ and the size is increasing exponentially with base 2. The one-step algorithm produces a linear generator with components $g_d = 2d - 1$ and a linearly increasing size $n = 6d - 4$.

For inference on the whole parameter vector, we observe again that the minimum power generator produces an exponentially increasing size with base 3. An iterative sequence of generator components is defined by the Fibonacci-type recursion

$$g_d = 2g_{d-1} + g_{d-2} + 1,$$

with initial values $g_1 = 1$, $g_2 = 3$. Hence, $g_d = ((1+\sqrt{2})^{d+1} + (1-\sqrt{2})^{d+1} - 2)/4$ by standard methods for nonhomogeneous linear recursions. This gives an approximate size $n \approx (1+\sqrt{2})^{d+1}/\sqrt{2}$ by the upper law.

Finally, the algorithm of Section 2.3 produces a one-step sequence of generator components which starts as follows:

$$(1, 3, 8, 18, 30, 43, 67, 90, 122, 161, \ldots)$$

and the corresponding sample sizes are $9, 23, 53, 97, 147, 221, 315, 425, 567, \ldots$ (for $d \geq 2$) obtained by the upper law.

3.2.2. *The model* $F(d; 2, \ldots, 2; 2)$. Next, we consider the complete two-factor interaction model $F(d; 2, \ldots, 2; 2)$ with marginal Fourier regressions of order 2, for which $n_{\max} = 2g_d + 2g_{d-1}$ and $n_3 = 2g_d$.

We start by making inference on the parameters associated with the main effects (including the constant term θ_0). This is the D_s-optimality mentioned in Section 2.2. The minimum power generator is given by

$$(g_1, \ldots, g_d) = (1, 5, 5^2, \ldots, 5^{d-1}),$$

with a size increasing exponentially with base 5.

A recursively defined, Fibonacci-type sequence of generator components is given by

$$g_d = 2g_{d-1} + 2g_{d-2} + 1,$$

with initial values $g_1 = 1$, $g_2 = 5$. This has solution $g_d = 2((1+\sqrt{3})^d + (1-\sqrt{3})^d - \frac{1}{2})/3$ and the sample size given by the generalized upper law for main effects equals approximately $n \approx 2(1+\sqrt{3})^{d+1}/\sqrt{3}$ and increases exponentially in the dimension.

The one-step iterative sequence of generator components starts as follows:

$$(1, 5, 13, 17, 37, 41, 49, 53, 109, 113, 121, 125, \ldots). \tag{5}$$

For this sequence the iterative generating law was found

$$g_d = g_{d-1} + 4\alpha_{d-1},$$

with $g_1 = 1$ and

$$\alpha_{2^j} = 3\alpha_{2^{j-1}} - 1,$$

with $\alpha_1 = 1$ and

$$\alpha_k = \alpha_{2^j} \quad \text{for } k = 2^j q,\ q \text{ odd}.$$

The next terms in the sequence are $145, 149, 157, 161, 325, 329$ given by both the one-step algorithm and the iterative sequence. The difference sequence α_k, $k = 1, 2, \ldots,$ gives

$$1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 41,$$

$$1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 122,$$

$$1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 41,$$

$$1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 365, \ldots,$$

which shows a nice self-similar structure. It can be proved that the iterative sequence produces suitable generators. Standard methods yield the solution $\alpha_{2^j} = \frac{1}{2}(3^j + 1)$ and $g_{2^j+1} = 4 \cdot 3^j + 1$. This, finally, implies that g_d increases

like d^γ where $\gamma = (\log 3)/(\log 2) \approx 1.5850$. The number $\gamma^{-1} = (\log 2)/(\log 3)$ is the Hausdorff dimension of the Cantor set and the reason for this unexpected connection can be seen by studying the structure of the sequence.

For inference on the whole parameter vector, the minimum power generator produces a size which increases exponentially with base 5. Alternatively, we present the following Fibonacci-type sequence of generator components

$$g_d = 4g_{d-1} + 2g_{d-2} + 1,$$

with initial values $g_1 = 1$, $g_2 = 5$. Hence, the generator sequence is $g_d = ((3+2\sqrt{6})(2+\sqrt{6})^d + (3-2\sqrt{6})(2-\sqrt{6})^d - 6)/30$ and the size is approximately equal to $(4+\sqrt{6})(2+\sqrt{6})^d/5$ by the upper law.

We finish this section with the one-step sequence of generator components

$$(1, 5, 23, 60, 77, 173, 222, 409, 535, 634, 935, 1182, 1361, 1497, \ldots) \tag{6}$$

and the corresponding sizes $25, 113, 333, 549, 1001, 1581, 2525, 3777, 4677, 6277, 8469, 10173, 11533, \ldots$ for $d \geq 2$ obtained by the upper law.

3.2.3. *The general model* $F(d; m, \ldots, m; 2)$. Finally, we investigate the two-factor interaction model $F(d; m, \ldots, m; 2)$ with marginal Fourier models of order m, for which $n_{\max} = m(g_d + g_{d-1})$ and $n_3 = mg_d$.

Again, we start by making inferences on the main effects. The minimum power generator given by $(1, (2m+1), \ldots, (2m+1)^{d-1})$ produces a size which is exponentially increasing with base $2m+1$. The following iterative, Fibonacci-type sequence:

$$g_d = m(g_{d-1} + g_{d-2}) + 1,$$

with initial values $g_1 = 1$, $g_2 = 2m + 1$ gives

$$g_d \approx \frac{m}{2m-1}\left(1 - \frac{m-2}{\sqrt{m^2+4m}}\right)\left(\frac{m+\sqrt{m^2+4m}}{2}\right)^d$$

and by the generalized upper law for main effects the sizes

$$n \approx \frac{m^2}{2m-1}\left(3 + \frac{5m+2}{\sqrt{m^2+4m}}\right)\left(\frac{m+\sqrt{m^2+4m}}{2}\right)^{d-1}$$

increase exponentially in the dimension.

In generalization of the case $m = 2$, we obtain another iterative sequence of generator components which is increasing at most polynomially:

$$g_d = g_{d-1} + 2m\alpha_{d-1},$$

with initial value $g_1 = 1$ where

$$\alpha_{2^j} = (m+1)\alpha_{2^{j-1}} - 1,$$

with initial value $\alpha_1 = 1$ and

$$\alpha_k = \alpha_{2^j} \quad \text{for } k = 2^j q,\ q \text{ odd}.$$

The difference sequence again shows a self-similar structure. As before, we obtain

$$\alpha_{2^j} = \frac{(m-1)(m+1)^j + 1}{m} \quad \text{and} \quad g_{2^j} = 2m(m+1)^j + 1.$$

This implies that g_d increases like d^γ where $\gamma = \log(m+1)/(\log 2)$. However, for $m > 2$ the iterative sequence differs from the sequence generated by the one-step algorithm.

Turning to inference on the whole parameter vector, for the minimum power generator we obtain the size

$$2m(g_d + g_{d-1}) + 1 = 4m(m+1)(2m+1)^{d-2} + 1$$

by the upper law. An iterative sequence of generator components is

$$g_d = m(2g_{d-1} + g_{d-2}) + 1,$$

with initial values $g_1 = 1$, $g_2 = 2m + 1$. Hence,

$$g_d \approx \frac{1}{3m-1}\left(\sqrt{\frac{m}{m+1}} + \frac{1}{2}\right)\left(m + \sqrt{m(m+1)}\right)^d,$$

with the approximate size

$$n \approx \frac{m}{3m-1}\left(2 + \sqrt{\frac{m+1}{m}}\right)\left(m + \sqrt{m(m+1)}\right)^d.$$

We conclude our presentation with some figures representing the behavior of the one-step generator sequence for the two-factor interaction models, both for inference on the main effects and on the whole parameter vector.

For the main effects in $F(d; 2, \ldots, 2; 2)$, Figure 1 shows the logarithm of α_d, the first differences of the generators divided by 4, over the dimension d for the sequence (5) up to $d = 180$. The self-similar structure mentioned previously is again evident. Figure 2 shows the logarithm of the generator of the same sequence over $\log(d)$ and gives an estimated slope of 1.7.

For inference on the whole parameter vector in $F(d; 2, \ldots, 2; 2)$, Figure 3 shows the logarithm $\log(g_d)$ of the generators for the one-step sequence (6) over the logarithm $\log(d)$ of the dimension giving an estimated slope of $\gamma \approx 2.72$. We have been unable to find an iterative sequence which yields this sequence or to link it to a Cantor-like set. The two log–log plots indicate polynomial growth d^γ of the size n in d with γ approximately equal to the estimated slopes. Note that the estimate 1.7 for the analysis of the main effects slightly overestimates $\gamma = (\log 3)/(\log 2) \approx 1.5850$.

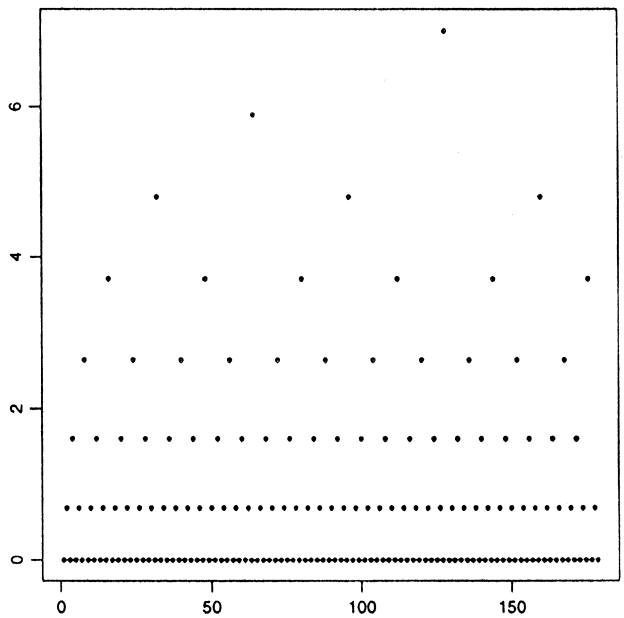

FIG. 1. *Main effect of the model* $F(d; 2, \ldots, 2; 2)$: $\log(\alpha_d)$ *over* d.

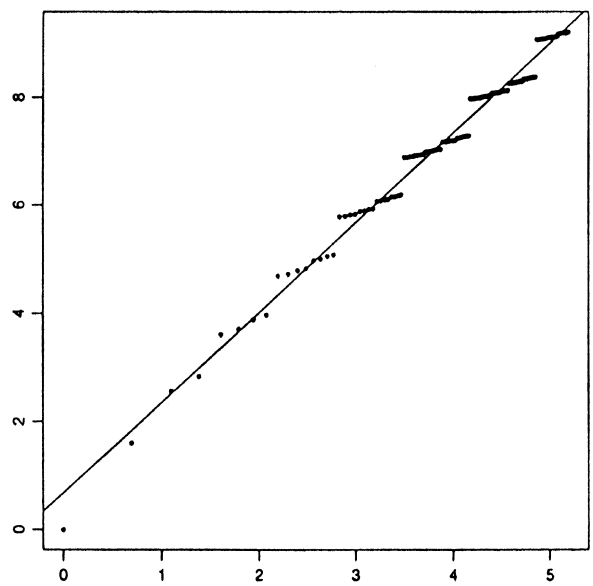

FIG. 2. *Main effect of the model* $F(d; 2, \ldots, 2; 2)$: $\log(g_d)$ *over* $\log(d)$.

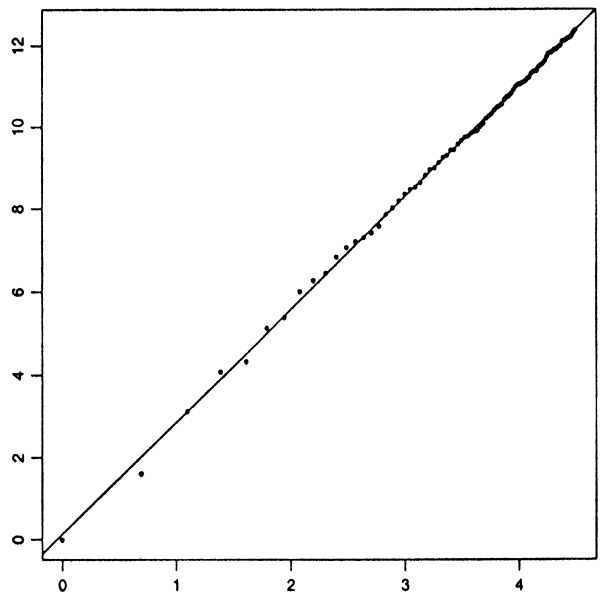

FIG. 3. *All effects of the model* $F(d; 2, \ldots, 2; 2)$: $\log(g_d)$ *over* $\log(d)$.

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