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THE USE OF LATTICES IN THE DESIGN OF HIGH-DIMENSIONAL EXPERIMENTS

RONALD A. BATES, EVA RICCOMAGNO, RAINER SCHWABE AND HENRY P. WYNN

University of Warwick, University of Warwick, University of Mainz and University of Warwick

In this paper we present a review of the theory of lattice designs for high dimensional experiments. In particular we consider space filling designs that are equally distributed, supported on one generator integer grid and are orthogonal for Fourier models. Those designs that are orthogonal for a larger class of Fourier models have better space filling properties leading to the idea of a "fan" of a lattice design.

1. Introduction. The dependence of the response of a statistical experiment on a set of explanatory variables can be described by a response surface, that is a general class of regression models of the type

$$Y(\boldsymbol{x}) = \mu(\boldsymbol{x}) + \varepsilon(\boldsymbol{x})$$

with multi-dimensional input $\boldsymbol{x} = (x_1, \ldots, x_d) \in [0,1[^d$, where ε is a random error and μ is the mean response, defined by

$$E\left(Y(\boldsymbol{x})\right) = \mu(\boldsymbol{x}).$$

Several observations $Y_1, \ldots, Y_N$ are taken at sites $\boldsymbol{x}_i$ $(i = 1, \ldots, N)$, and the fitted model $\hat{\mu}$ is meant to minimize the distance to the true response. For example this distance can be measured by the integrated mean squared error.

In case of complete ignorance of the structure of the response μ and when homoscedasticity is assumed, it is natural to take equally spaced observations [for asymptotic results in the setting of random designs see Ruppert and Wand (1994), for the general situation or Opsomer and Ruppert (1997), in the presence of an additive structure. Indeed the homoscedastic case which is of interest here can be obtained by considering a constant variance function.] See Müller (1984) for the heteroscedastic case. It is desirable that also the one-dimensional projections are equally spaced in order to obtain good marginal properties. In particular the projections onto the axes should have as many points as the design. For example the designs in column c) of Figure 1 are to be preferred to those in columns a) and b).

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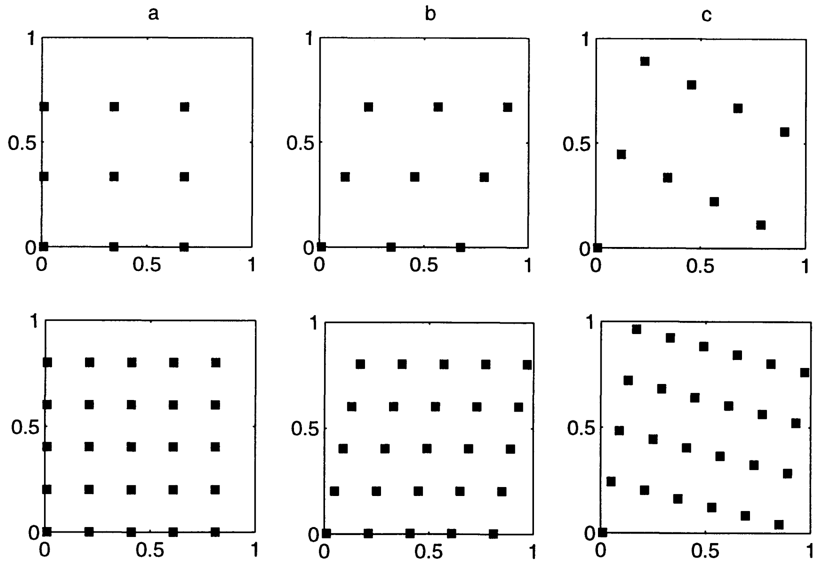

FIG. 1. *Examples of lattice designs with* 9 *and* 25 *points.*

2. Integration lattices. Integration lattices have been widely used in integration theory for their space filling properties and the possibility to impose regular one-dimensional projections, that is the projections are equally spaced [see Niederreiter (1992) and Sloan and Joe (1994)]. They are used as supporting points for quadrature formulae for one-periodic functions over the unitary hypercube $[0,1[^d$. We recall that a function f is one-periodic in each component if $f(\boldsymbol{x}) = f(\boldsymbol{x}+\boldsymbol{c})$ for all vectors $\boldsymbol{c}$ with integer components.

A finite integration lattice is a subset of $[0,1[^d$ which has a group structure with respect to the sum modulo 1, that is the summation is jointly applied with the "fractional part" operation. Note that the fractional part of the vector $\boldsymbol{x}$ is the vector

$$\{\boldsymbol{x}\} = (x_1 \,(\mathrm{mod}\ 1), \dots, x_d \,(\mathrm{mod}\ 1)).$$

Lattices can be written in a canonical form as follows [see Sloan and Joe (1994)]. For any lattice L there exists a unique positive integer r called *rank.* Moreover there exist r linearly independent integer vectors (*generators*) $\boldsymbol{g}_1, \dots, \boldsymbol{g}_r$ and unique r positive integers (*invariants*) $N_1, \dots, N_r$ satisfying $N_{\varrho+1}$ divides N_ϱ for all $\varrho = 1, \dots, r-1$ such that the lattice can be written as follows:

$$\left\{\left\{k_1 \frac{\boldsymbol{g}_1}{N_1} + \cdots + k_r \frac{\boldsymbol{g}_r}{N_r}\right\} : k_1 = 0, \dots, N_1 - 1, \dots, k_r = 0, \dots, N_r - 1\right\}.$$

The numbers of distinct points in the lattice equals $N = N_1 \cdot \ldots \cdot N_r$. The lattice generated by the vectors $\boldsymbol{g}_1, \dots, \boldsymbol{g}_r$ with invariants $N_1, \dots, N_r$ is indicated by $L_{\boldsymbol{g}_1,\dots,\boldsymbol{g}_r;N_1,\dots,N_r}$.

Notice that the first generator "holds" most of the lattice points. This leads us to favor rank one or one-generator lattices. In order to get regular projections onto the axes we require that the greatest common divisor of the number of lattice points and the coordinates of the generator is one. In this case we may assume the first coordinates of one-generator lattices equal to 1, which can be accomplished by a relabeling of the sites. To be more precise, the lattice generated by $\boldsymbol{g} = (g_1, \ldots, g_d) \in \mathbb{Z}^d$ and with N points is given by the following rule:

$$\begin{aligned} L_{g;N} &= \left\{ \left\{ \frac{k\boldsymbol{g}}{N} \right\}; k = 0, \ldots, N-1 \right\} \\ &= \left\{ \left(\frac{kg_1 \bmod N}{N}, \ldots, \frac{kg_d \bmod N}{N} \right); k = 0, \ldots, N-1 \right\}. \end{aligned}$$

A one-generator lattice can be visualised as a set of points on a trajectory embedded in $[0,1[^d$ interpreted as the d-dimensional torus.

The designs in column a) of Figure 1 are the rank two lattices $L_{(1,0),(0,1);3,3}$ and $L_{(1,0),(0,1);5,5}$. The second column presents the one-generator lattices $L_{(1,3);9}$ and $L_{(1,5);25}$. In the third column the one-generator lattices $L_{(1,4);9}$ and $L_{(1,6);25}$ are shown which have the additional nice feature of regular projections onto both axes.

3. Fourier approximation. To judge the performance of a design we require that it is suitable (or even optimal) for a certain (parametric) class of functions. Due to the periodicity property it is appropriate to choose Fourier (trigonometric) models which fall naturally in the category of one-periodic functions as approximations to a response surface model. This is motivated for example by the discrete Fourier transform used in various areas of engineering [see Bracewell (1978)]. A general Fourier model is defined via a finite set of frequencies $A \subset \mathbb{Z}^d$ as follows:

$$\mu(\boldsymbol{x}) = E(Y(\boldsymbol{x})) = \theta_0 + \sqrt{2} \sum_{h \in A;\, h \neq 0} \left[\theta_h \sin(2\pi \boldsymbol{h}^t \boldsymbol{x}) + \phi_h \cos(2\pi \boldsymbol{h}^t \boldsymbol{x}) \right] \;,$$

where $\boldsymbol{x} \in [0,1[^d$ and θ_0, θ_h and ϕ_h are real parameters for all $\boldsymbol{h} \in A$. As usually the set A of frequencies is assumed to be *symmetric*, that is $\boldsymbol{h} \in A$ implies $-\boldsymbol{h} \in A$, and the model is overparameterized in the general case $A \neq \{0\}$. Therefore we give a minimal (not unique) parameterization in terms of a set of $A_0 \subset \mathbb{Z}^d$ such that (i) $0 \notin A_0$ and (ii) if $\boldsymbol{h} \in A_0$ then $-\boldsymbol{h} \notin A_0$ so that $A = A_0 \cup (-A_0) \cup \{0\}$. If m is the number of elements in A_0 then the model has $p = 2m + 1$ parameters.

In several situations we require that A is *complete*, that is the frequency set has an "order ideal" structure in the following sense. If the frequency $\boldsymbol{h} = (h_1, \ldots, h_d)$ is in A then all frequencies $\boldsymbol{a} = (a_1, \ldots, a_d)$ which satisfy $|a_i| \leq |h_i|$ (for $i = 1, \ldots, d$) are in A. In particular, this implies that for every frequency $\boldsymbol{h} = (h_1, \ldots, h_d)$ all symmetric images $(z_1 h_1, \ldots, z_d h_d)$ with $z_1, \ldots, z_d \in \{-1, 1\}$ are included, the latter being a natural condition arising from the interpretation of $\boldsymbol{h}^t \boldsymbol{x}$ as an interaction term of the marginals $|h_i| x_i$ for the non-zero components h_i, $i = 1, \ldots, d$. For these complete models we define the generator A^+ of the model with frequency set A as the set of all non negative frequencies in A, that is

$$A = \left\{ \boldsymbol{h} : (|h_1|, \ldots, |h_d|)^t \in A^+ \right\}.$$

For example if $(1,1)$ is in A^+ then the frequencies $(1,-1), (-1,1)$ and $(-1,-1)$ are in A.

A particular important class of complete models is given by the M-factor interaction models $F(d; m_1, \ldots, m_d; M)$ where d denotes the number of factors, m_i is the degree of the Fourier regression for the ith factor and M is the maximum number of factors in an interaction involved. For these models the generating set A^+ of frequencies is given by

$$A^+ = \{\boldsymbol{h} : 0 \leq h_i \leq m_i, \text{ and } h_i \neq 0 \text{ for at most } M \text{ components}\}.$$

For one-dimensional models $F(1; m; 1)$ it is known [see Kiefer and Wolfowitz (1959)] that equally spaced designs with at least $p = 2m + 1$ points produce diagonal information matrices. The one-generator lattice designs generalise this concept. They are equally spaced designs on a line wrapped around the $(d+1)$-dimensional unitary torus. By suitably exploiting these properties the identifiability of a high-dimensional Fourier model is reduced to the study of a one-dimensional (non-complete) Fourier model [see Riccomagno, Schwabe and Wynn (1997)]. Note that when considering one-generator lattices the uniform (Lebesgue) measure on the one-dimensional "subspace" generated by the "direction" of the generator $\boldsymbol{g}$ (slope) bears the same information matrix and is hence optimal. In contrast to traditional methods [see for example Rafajłowicz and Myszka (1992) and Schwabe (1996)] the main idea here is that first a reduction of the dimension (to one) is performed and after that the problem is discretised by choosing an equally spaced design on the one-dimensional subspace. This theory carries over to rank r lattices. Note that the full factorial design with $2m_i + 1$ levels at the ith factor (for all $i = 1, \ldots, d$), which is orthogonal for the Kronecker product-type complete d-factor interaction model $F(d; m_1, \ldots, m_d; d)$, is the full rank lattice generated by the unit vectors $\boldsymbol{e}_i$ $(i = 1, \ldots, d)$ with $N_i = 2m_i + 1$.

Due to the lattice structure in conjunction with the orthogonality property of trigonometric functions on a uniform grid the design $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ is either orthogonal, that is the standardised information matrix equals the identity, or it is rank deficient. As the model is not identifiable in the latter case identifiability orthogonality is automatically implied by orthogonality. Moreover, orthogonal designs are simultaneously D-, A-, E- and $IMSE$-optimal for a true trigonometric response μ. More generally, orthogonal designs are universally optimal in the sense of Kiefer (1975) [see Pukelsheim (1993, Chapter 14)]. A design which is orthogonal for a model with frequency set A is also orthogonal for any submodel with frequency set $A' \subset A$. In particular, orthogonality for a M-factor interaction model $F(d; m_1, \ldots, m_d; M)$ implies orthogonality for each K-factor interaction model $F(d; k_1, \ldots, k_d; K)$ when $k_i \leq m_i$ $(i = 1, \ldots, d)$ and $K \leq M$.

4. Dual lattices and identifiability. The dual of a lattice is a powerful tool to characterise the identifiability of a Fourier model.

DEFINITION 1. *The dual lattice $L^{\perp}$ of a lattice L is defined as*

$$L^{\perp} = \left\{ \boldsymbol{h} \in \mathbb{Z}^d \text{ such that } \boldsymbol{h}^t\boldsymbol{x} \in \mathbb{Z} \text{ for all } \boldsymbol{x} \in L \right\}.$$

For a one-generator lattice $L_{g;N}$ the definition of a dual lattice simplifies to

$$L^{\perp}_{g;N} = \left\{ \boldsymbol{h} \in \mathbb{Z}^d \text{ such that } \boldsymbol{h}^t\boldsymbol{g} \equiv 0 \pmod N \right\}.$$

The dual lattice $L^{\perp}_{g;N}$ is the orthogonal subspace to the standardised lattice $N \cdot L$ (with respect to the scalar product in $\mathbb{Z}^d$ modulo N). For the lattice $L_{(1,2);5}$ the dual lattice is an integer grid generated by $(1,2)$ and $(0,5)$, that is $L^{\perp}_{(1,2);5} = \{(k, 2k+5j) : j,k \in \mathbb{Z}\}$.

The dual lattice of a rank r lattice generated by $\boldsymbol{g}_1, \dots, \boldsymbol{g}_r$ with invariants $N_1, \dots, N_r$ is the set of integer vectors that satisfy the following system of equations

$$\begin{cases} \boldsymbol{h}^t\boldsymbol{g}_1 & \equiv & 0 \pmod{N_1}; \\ & \vdots & \\ \boldsymbol{h}^t\boldsymbol{g}_r & \equiv & 0 \pmod{N_r}. \end{cases}$$

For example the dual lattice of the full rank lattice in two dimensions with generators $\boldsymbol{g}_1 = (1,0)$ and $\boldsymbol{g}_2 = (0,1)$ and with 9 points is given by

$$L^{\perp}_{g_1,g_2;3,3} = 3\mathbb{Z}^2 = \{(3h_1, 3h_2) : \ h_1, h_2 \in \mathbb{Z}\}.$$

In both above examples it can be recognized that the dual lattice has the same spatial structure as the lattice itself but under a larger scale. However, this is not the case for all lattices.

As a further example consider the one-generator lattice in three dimensions generated by $\boldsymbol{g} = (1,2,3)$ with 7 points. The dual lattice is generated by the vectors $(0,1,4)$ and $(1,0,2)$ on the region $[0,7[^3$ and it contains 49 points within that region, that is

$$L^{\perp}_{g;7} \cap [0,7[^3 = \{j(0,1,4) + k(1,0,2) \pmod 7 : j,k \in \mathbb{Z}\}.$$

Moreover the two-dimensional projections of the dual lattice are regular. The structure of the dual lattice allows us to estimate a variety of different models.

Indeed dual lattices govern the aliasing structure of a Fourier model/lattice design pair in the sense of the following theorems. Necessary and sufficient conditions are given for a pair of frequencies $(\boldsymbol{h}_1, \boldsymbol{h}_2)$ to be mutually orthogonal, that is they can be included in the same identifiable model. This condition is similar to the condition of not being aliased in a factorial experimental design. In the same spirit the generators of the dual lattice describe the aliasing structure in a similar way as it is done by the defining sequences in factorial experiments.

THEOREM 1. *The Fourier model given by the set of frequencies A is identifiable by the rank r generator lattice $L_{g_1,\dots,g_r;N_1,\dots,N_r}$ if and only if for every $\boldsymbol{k} = (k_1, \dots, k_r) \in \mathbb{Z}^r$ satisfying $0 \le k_i \le N_i - 1$ $(i = 1, \dots, r)$ there exists at most one $\boldsymbol{h} \in A$ such that*

$$\begin{aligned} &\boldsymbol{h}^t\boldsymbol{g}_1 \equiv k_1 \pmod{N_1}; \\ &\vdots \\ &\boldsymbol{h}^t\boldsymbol{g}_r \equiv k_r \pmod{N_r}; \end{aligned}$$

The proof of this theorem relies on a generalisation of the simple fact that the sum of sinusoidal functions over the N complex roots of the unity has value zero [see Sloan and Joe (1994, Lemma 2.1) and Niederreiter (1992, Lemma 5.21) for a proof based on the group representation of lattices]. For details see Riccomagno, Schwabe and Wynn (1997).

Note that the Fourier model defined by the set of frequencies A is identifiable by a generator lattice L if each frequency $\boldsymbol{h}$ in A belongs to a different coset of $L^{\perp}$.

TABLE 1

Complete models identifiable by $L_{(1,2),5}$

	(i)	(ii)	(iii)
A_0	(1,0)	(1,0)	(0,1)
	(2,0)	(0,1)	(0,2)
p	5	5	5

TABLE 2

Complete models identifiable by $L_{(1,5),13}$

	(i)	(ii)	(iii)	(iv)	(v)	(vi)	(vii)
A_0	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(0,1)
	(2,0)	(2,0)	(2,0)	(2,0)	(0,1)	(0,1)	(0,2)
	(3,0)	(3,0)	(3,0)	(0,1)	(0,2)	(0,2)	(0,3)
	(4,0)	(4,0)	(0,1)	(0,2)	(0,3)	(0,3)	(0,4)
	(5,0)	(0,1)	(1,1)	(1,1)	(1,1)	(0,4)	(0,5)
	(6,0)		(1,-1)	(1,-1)	(1,-1)		(0,6)
p	13	11	13	13	13	11	13

Table 1 gives all the maximal (with respect to the inclusion) complete models identifiable by $L_{(1,2),5}$. The lattice $L_{(1,5),13}$ can be used to fit the maximal complete models given in Table 2. Notice there that the factors are treated symmetrically by the lattice and that the models (ii) and (vi) are not saturated.

Table 3 presents the list of all maximal complete models estimable with the nine point designs of Figure 1. The first column gives the only complete model identifiable by $L_{(1,0),(0,1);3,3}$ as known from standard theory. In the second block there are those complete models which are identifiable by $L_{(1,3);9}$. The third block gives the set of models identifiable by $L_{(1,5);9}$. We could refer to those blocks by the term of the *fan* of the corresponding design, in the sense that they represent the full range of complete models identifiable by the design [see Caboara, Pistone, Riccomagno and Wynn (1997) for a recent reference to the notion of fan in experimental design]. Thus the bigger the fan is the better space filling properties the design has.

TABLE 3

Complete models identifiable by designs with 9 points in Figure 1

	a)	b)			c)		
	(i)	(i)	(ii)	(iii)	(i)	(ii)	(iii)
A^+	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(0,1)
	(0,1)	(2,0)	(2,0)	(0,1)	(2,0)	(2,0)	(0,2)
	(1,1)	(3,0)	(0,1)	(1,1)	(3,0)	(3,0)	(0,3)
		(4,0)			(4,0)	(0,1)	(0,4)
p	9	9	7	9	9	9	9

TABLE 4

Complete models identifiable by designs with 25 points in Figure 1

	a)	b)				c)				
	(i)	(i)	(ii)	(iii)	(iv)	(i)	(ii)	(iii)	(iv)	(v)
A^+	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(1,0)	(0,1)
	(2,0)	(2,0)	(2,0)	(2,0)	(2,0)	(2,0)	(2,0)	(2,0)	(2,0)	(0,2)
	(0,1)	(3,0)	(3,0)	(3,0)	(0,1)	(3,0)	(3,0)	(3,0)	(3,0)	(0,3)
	(0,2)	(4,0)	(4,0)	(0,1)	(0,2)	(4,0)	(4,0)	(4,0)	(0,1)	(0,4)
	(1,1)	(5,0)	(0,1)	(0,2)	(1,1)	(5,0)	(5,0)	(0,1)	(0,2)	(0,5)
	(2,1)	(6,0)	(0,2)	(1,1)	(2,1)	(6,0)	(0,1)	(0,2)	(1,1)	(0,6)
	(1,2)	(7,0)		(1,2)	(1,2)	(7,0)	(0,2)	(1,1)	(2,1)	(0,7)
	(2,2)	(8,0)			(2,2)	(8,0)	(0,3)			(0,8)
		(9,0)				(9,0)				(0,9)
		(10,0)				(10,0)				(0,10)
		(11,0)				(11,0)				(0,11)
		(12,0)				(12,0)				(0,12)
p	25	25	13	19	25	25	17	17	19	25

Similarly Table 4 refers to the 25 point designs $L_{(1,0),(0,1);5,5}$, $L_{(1,5);25}$ and $L_{(1,6);25}$ of Figure 1. If we are only interested in additive models $F(2; m_1, m_2; 1)$ in which only frequencies of the type $(h_1, 0)$ and $(0, h_2)$ occur, then the lattices $L_{(1,4);9}$ and $L_{(1,6);25}$ do not only have regular projections but they also outperform their competitors by covering a larger fan of models. Note also that for the one-generator designs in columns b) and c) the factors are not treated symmetrically.

Figure 2 explains the mechanism behind Theorem 1. The first graph gives the dual lattice of $L_{(1,2);5}$ on the grid $[-5,5[^2 \cap \mathbb{Z}^2$. The second and third show the cosets which are added by including $+x_1$ and $-x_1$ in the identifiable model. And finally the third one represents the cosets associated to $\pm x_2$. Hence, a maximal model identifiable by $L_{(1,2);5}$ is given by $A_0 = \{(1,0),(0,1)\}$.

As a further example consider the two-dimensional design on the rank two lattice

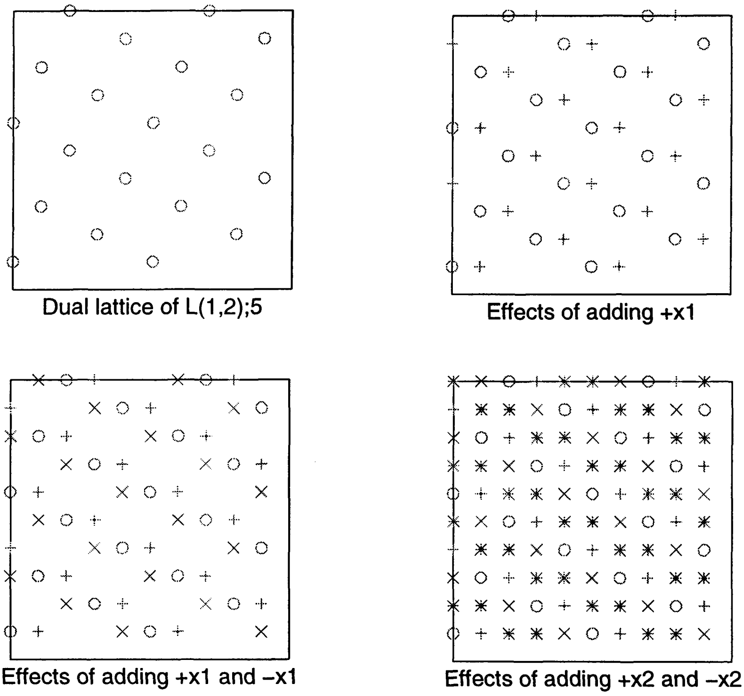

FIG. 2. *The dual lattice of* $L_{(1,2);5}$ *and the cosets corresponding to the first-order effects.*

generated by $\boldsymbol{g}_1 = (1,0)$, $N_1 = 2$ and $\boldsymbol{g}_2 = (1,1)$, $N_2 = 4$. So that

$$L = \left\{ \frac{k(2,0) + \ell(1,1)}{4} \;:\; k = 0,1, \quad \ell = 0,1,2,3 \right\}$$

gives the 8-point design $(0,0), (\frac{1}{4},\frac{1}{4}), (\frac{1}{2},\frac{1}{2}), (\frac{3}{4},\frac{3}{4}), (\frac{1}{2},0), (\frac{3}{4},\frac{1}{4}), (0,\frac{1}{2}), (\frac{1}{4},\frac{3}{4})$, which is the union of two 2^2 full-factorials —one at levels 0 and $\frac{1}{2}$ and the other at levels $\frac{1}{4}$ and $\frac{3}{4}$. The set $A_0 = \{(0,1),(1,0)\}$ defines the maximal complete Fourier model identifiable by L.

A major research effort is to determine the fan of a design in an automatic way and to possibly obtain a classification of designs according to the structure of their fan.

5. Complexity. The challenge of the theory is to determine automatic sequences of orthogonal design for a natural class of complete Fourier models as the dimension increases. Riccomagno, Schwabe and Wynn (1997) consider the problem for additive and two-factor interaction models and determine designs whose sample size increases polynomially with the dimension, while usually there is an exponential increase for product-type designs or designs obtained by Fibonacci-type recursions applied to the components of the generator sequence. In particular a complexity theory is proposed in which the size of the design in compared with some descriptor of the model such as the dimension d or the number of parameters p. Given a model $F(d; m_1, \ldots, m_d; M)$

and a suitable generator sequence $(g_i)_{i=1,\ldots,d}$ the sample size is computed as

$$2 \max_{i=1,\ldots,d} m_i g_i + 1.$$

Thus a bound on the generator sequence gives a bound on the sample size as d increases.

For the example of the additive models $F(d; m, \ldots, m; 1)$ the one-generator lattice designs generated by $(1, m+1, 2m+1, \ldots)$ with sample size $2m^2(d-1) + 2m + 1$ are orthogonal with the sample sizes increasing linearly in the dimension d.

For the two interaction model $F(24; 1, \ldots, 1; 2)$ the following generator sequence gives an orthogonal design

$$1, 3, 8, 18, 30, 43, 67, 90, 122, 161, 202, 260, 305, 388, 416,$$
$$450, 555, 624, 730, 750, 983, 1059, 1159, 1330.$$

In Figure 3 the logarithm of g_d is plotted against $\log d$, for $d > 1$, showing that g_d increrases like $d^{2.43}$.

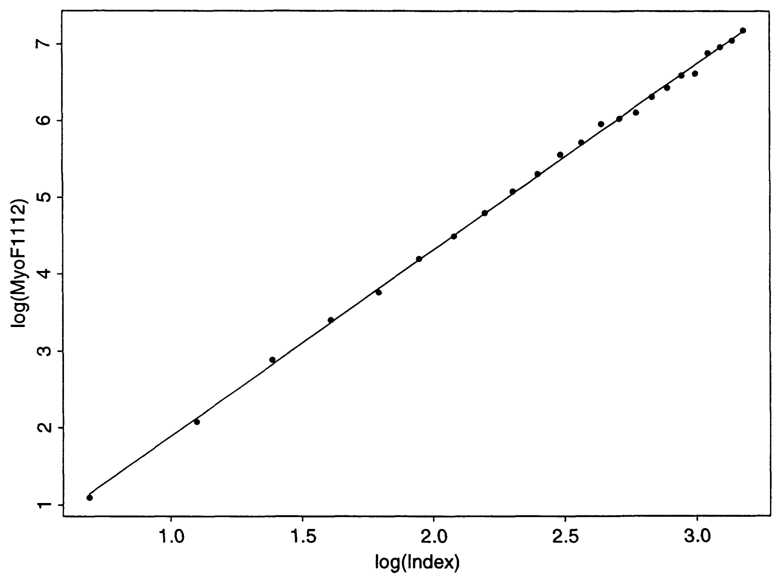

FIG. 3. log-log *plot for* $F(d; 1, \ldots, 1; 2)$ $(d > 1)$.

Analogously Riccomagno, Schwabe and Wynn (1997) obtain a sequence that behaves like $d^{2.72}$ for the identification of all parameters in the models $F(d; 2, \ldots, 2; 2)$. For the identification of the main effects (Resolution IV) in the same model $F(d; 2, \ldots, 2; 2)$ they obtain an explicit formula for the generator sequence which increases in the dimension like $d^{\log 3/\log 2}$.

In conclusion, we have seen that lattice designs and in particular one-generator lattice designs have good space filling properties with regular projections and are orthogonal for proper Fourier models. The aliasing structure follows nicely from the general theory. For special classes of Fourier models it is possible to find sequence of designs whose sample size incresaes polynomially with the dimension. It is possible to discriminate among designs according to how many and what kind of models they identify (fan theory).

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RONALD A. BATES, EVA RICCOMAGNO
AND HENRY P. WYNN
DEPARTMENT OF STATISTICS
UNIVERSITY OF WARWICK
COVENTRY CV4 7AL
UNITED KINGDOM

RAINER SCHWABE
MATHEMATISCHES INTITUT
FREIE UNIVERSITÄT BERLIN
ARNIMALLEE 2-6
D-14195 BERLIN
GERMANY