

A Thesis Submitted for the Degree of PhD at the University of Warwick

Permanent WRAP URL:

<http://wrap.warwick.ac.uk/133951>

Copyright and reuse:

This thesis is made available online and is protected by original copyright.

Please scroll down to view the document itself.

Please refer to the repository record for this item for information to help you to cite it.

Our policy information is available from the repository home page.

For more information, please contact the WRAP Team at: wrap@warwick.ac.uk

Algebraic Geometry in Experimental Design and Related Fields

Eva M. Riccomagno

This thesis is submitted for the degree of Doctor of Philosophy

Department of Statistics
University of Warwick
Coventry
CV4 7AL

August 1997

Contents

1	Introduction	1
I	Gröbner Bases in Experimental Design	7
2	Introduction to Gröbner bases	9
2.1	Polynomials and polynomial ideals	9
2.1.1	Orderings	11
2.1.2	Division	14
2.1.3	Division algorithm	15
2.1.4	Hilbert basis theorem	16
2.2	Varieties	18
2.3	Gröbner bases and the Buchberger algorithm	20
2.3.1	The Buchberger algorithm	22
2.4	Elimination theory	24
2.5	Polynomial functions and quotients by ideals	25
3	Design varieties and identifiability	29
3.1	The design variety	29
3.1.1	Examples	31
3.2	Algebraic identifiability	34
3.2.1	Examples	36
3.3	The fan of a design	41
3.3.1	Interpolation	44
3.4	The model ideal	47
II	Fourier Models and Lattice Designs	53
4	Generalities for Fourier models and lattice grids	55
4.1	Fourier models	55
4.1.1	Examples of Fourier models	59
4.2	Optimum designs: background	63
4.3	Lattice designs	65
4.3.1	Multirank lattices	68
4.3.2	The error for quadrature formulae based on lattices	71

5	Orthogonality of lattice designs for Fourier models	73
5.1	Motivation	74
5.2	Another example: complete interaction models	75
5.3	Complete models	76
5.4	Mutually orthogonal frequencies	77
5.5	Double cosets	78
5.6	Orthogonality of multirank lattices for Fourier models	81
6	Finding good generators	85
6.1	Generator prototypes	85
6.2	Sample size	91
6.3	Additive models	92
6.3.1	Power type generators	92
6.3.2	Recursively defined generators	93
6.3.3	One-step generators and linear generators	97
6.4	Two-factor interaction models	97
6.4.1	The models $F(d; 1, \dots, 1; 2)$	99
6.4.2	The models $F(d; 2, \dots, 2; 2)$	101
6.4.3	The models $F(d; m, \dots, m; 2)$	104
7	Lattice designs for screening experiments	115
7.1	Analysis of a known function	118
7.2	The fitted model	120
III	Algebraic Identifiability for Fourier Models	133
8	Applications of Gröbner bases to Fourier models	135
8.1	Fourier models as polynomials	135
8.2	Polynomial representation of lattice designs	138
8.3	Gröbner basis technology	139
8.4	Examples	141
8.4.1	Example: $L_{(1,5),13}$	141
8.4.2	Example: the union of $L_{(1,5),13}$ and D	143
8.4.3	Example: the design F	144
IV	Conclusions and Further Research	149
V	Appendices	159
.1	Computer algebra packages	161
.2	Buchberger algorithm for complex numbers	163

List of Figures

2.1	Example of order ideal.	17
4.1	Frequency set for the additive model $m_1 = 4, m_2 = 2$	61
4.2	Frequency set for $F(2; 4, 2; 2)$	62
5.1	Lattice generated by $g_1 = (2, 0), N_1 = 2$ and $g_2 = (1, 1), N_2 = 4$	82
6.1	Main effect of the model $F(d; 2, \dots, 2; 2): \log(\alpha_d)$ over d	108
6.2	Main effects of the model $F(d; 2, \dots, 2; 2): \log(g_d)$ over $\log(d)$	108
6.3	All effects of the model $F(d; 2, \dots, 2; 2); \log(g_d)$ over $\log(d)$	111
7.1	Observed values at the $L_{(1,5),13}$ design points.	124
7.2	Power spectrum augmented by the mean.	124
7.3	Observed values at the $L_{(1,5),16}$ design points.	125
7.4	Power spectrum augmented by the mean.	125
7.5	Observed values at $L_{(1,61,11),721}$ from $x_1^{x_3}$	126
7.6	Power spectrum for data from $x_1^{x_3}$	126
7.7	Frequencies with highest spectrum for data from $x_1^{x_3}$	126
7.8	Observed values at $L_{(11,61,1),721}$ from $x_1^{x_3}$ and power spectrum.	127
7.9	Power spectrum for data from $x_1^{x_3}$ at $L_{(11,61,1),721}$	127
7.10	Frequencies with highest spectrum for data from $x_1^{x_3}$	127
7.11	Observed values at $L_{(1,61,11),721}$ from $x_1^{x_3+1x_2}$	128
7.12	Power spectrum for values at $L_{(1,61,11),721}$ from $x_1^{x_3+1x_2}$	128
7.13	Frequencies with highest spectrum for data from $x_1^{x_3}$ at $L_{(1,61,11),721}$	128
7.14	Observed values at $L_{(11,61,1),721}$ from $x_1^{x_3+1x_2}$	129
7.15	Power spectrum for values at $L_{(11,61,1),721}$ from $x_1^{x_3+1x_2}$	129
7.16	Frequencies with highest spectrum for data from $x_1^{x_3}$	129
7.17	Observed values and power spectrum for the Welch et al. function.	130
7.18	Power spectrum for the Welch et al. function for the lattice design with $g_i = 2i - 1$ and $N = 134$	130
7.19	Frequencies with highest spectrum for the Welch et al. function.	131
7.20	Frequencies with highest spectrum for the Welch et al. function for the lattice design with $g_i = 3i - 2$ and $N = 207$	131

List of Tables

2.1	Division algorithm.	17
2.2	The algebra-geometry dictionary.	27
3.1	CoCoA macros for design ideals.	32
3.2	CoCoA macro for identifiability.	37
4.1	The dimension of some parameter vectors.	63
4.2	Optimality criteria.	64
6.1	Code for the one-step strategy for $F(d; m_1, \dots, m_d; 1)$	98
6.2	Code for the one-step strategy for the main effects of $F(d; m_1, \dots, m_d; 2)$	109
6.3	Code for the one-step strategy for all the effects of $F(d; m_1, \dots, m_d; 2)$	110
6.4	Linear type generator for the models $F(d; 2, \dots, 2; 1)$	111
6.5	Linear generator for the models $F(d; 3, \dots, 3; 1)$	111
6.6	Linear generator for the models $F(d; 4, \dots, 4; 1)$	111
6.7	One-step generator for the models $F(d; 2, \dots, 2; 1)$	112
6.8	One-step generator for the models $F(d; 3, \dots, 3; 1)$	112
6.9	One-step generator for the models $F(d; 4, \dots, 4; 1)$	112
6.10	Models with two-factor interaction and first order marginal.	112
6.11	Models with two-factor interaction and second order marginal.	113
6.12	Models with two-factor interaction and equal order marginal.	113
8.1	The design D	146
8.2	The design F	146
8.3	Estimable terms by $L_{(1,5),13} \cup D$	147

Notation

\mathbb{N} is the set of non negative integer numbers.

\mathbb{Z} is the set of integer numbers.

\mathbb{Q} is the set of rational numbers.

\mathbb{R} is the set of real numbers.

\mathbb{C} is the set of complex number.

A letter, usually d , as superscript represents the dimension of the cartesian product for example \mathbb{Z}^d stands for $\underbrace{\mathbb{Z} \times \dots \times \mathbb{Z}}_{d \text{ times}}$.

A $*$ superscript to a set excludes the 0 of the set, for example \mathbb{N}^* is the set of positive integers. While a $*$ superscript to a matrix A denotes the complex and conjugate matrix of A .

A t superscript to a matrix or a vector gives the transpose matrix or vector.

A $_+$ subscript to a set of numbers denotes the positive entries of the set, for example $\mathbb{Z}_+^* = \{a \in \mathbb{Z} : a > 0\}$.

E stands for expectation.

We do not denote vectors in any special way, for example in bold face. It will be clear that we are dealing with vectors by the context.

$\{a\}$ is the result of the fractional part operator where $a \in \mathbb{R}^d$ for $d \geq 1$ or the set whose element is a .

$\#(A)$ is the cardinality of the set A that is the number of elements of A .

\mathbb{N}_0 is the cardinality of the integer numbers, thus of the non-negative integers and of the rational numbers.

$\mathcal{N}_m := \{r : r = -1, \dots, -1, 0, 1, \dots, m\}$.

$\mathcal{N}_m^* := \{r : r = -1, \dots, -1, 1, \dots, m\}$.

\mathcal{G}_m is the additive group over $\{0, 1, \dots, m - 1\}$.

I is the identity matrix.

N is the sample size or the number of lattice points.

Acknowledgments

I would like to thank my supervisor Professor Henry Wynn and all those who helped and supported me in this period. A special thanks is due to Professor Giovanni Pistone who collaborated with Professor Wynn and myself during the period of this thesis. I am grateful to my ex-colleague Tim Holliday who carefully read the thesis and to my other coauthors Ron Bates, Massimo Caboara, Tim Holliday, Rainer Schwabe and Lisa White for teaching me so much. I would also like to thank the UK Engineering and Physical Science Research Council for the financial support under grants GR/K72247 (*Application of Algebraic Geometry to the Design of Experiments*), GR/K81737 and GR/H33572 (both titled *Experimental and inductive methods in statistical quality improvement*).

Declaration

I declare that this thesis is in part my work and in part collaboration with various coauthors. The part of this thesis on Fourier models and lattice designs started with the paper *Experimental design and observation for large systems (with discussion)* by Bates, Buck, Riccomagno and Wynn presented at the meeting on Experimental Design at the Royal Statistical Society on April 1995. This was followed by the paper titled *Lattice-based optimum design for Fourier regression* in collaboration with Schwabe and Wynn to appear on *The Annals of Statistics*. The paper *Lattices and Dual Lattices in Optimal Experimental Design for Fourier Models* was accepted for publication in *Computational Statistics and Data Analysis (CSDA)* and the technical report *Fast Fourier Emulators Based on Space-filling Lattices* was presented at ICIAM '95. Both works are in collaboration with Bates, Schwabe and Wynn.

The work on the application of Gröbner bases to experimental design was started by Pistone and Wynn with the paper *Generalised confounding with Gröbner bases* (*Biometrika*, 1996). The following papers include material from the present thesis: *The Application of Algebraic Geometry to the Analysis of Designed Experiments: A Case Study* (with Holliday, Pistone and Wynn, accepted for publication on *Computational Statistics*); *The fan of an experimental design* (with Caboara, Pistone and Wynn, submitted to *The Annals of Statistics*); *Computational Algebraic Geometry in Industrial Experimental Design* (with Wynn, in *The Proceedings of the International Conference on Industrial Statistics: Aims and Computational Aspects*, 1997); *An algebraic computational approach to the identifiability of Fourier models* (with Caboara, under revision for publication on the *Journal of Symbolic Computation*). At the beginning of the project Professor Wynn and I gave a series of four lectures at the Department of Statistics at Warwick University on the basics of Gröbner bases and their applications to experimental design and statistics. This work is being extended into a monograph in collaboration with Professor Pistone.

I have a major responsibility for the comprehensive reworking of the basic theory in Chapter 3 and the new work particularly Sections 3.3 and 3.4. In Chapters 4 and 5 I worked on the basic theory. Section 5.6 is my own work and I worked extensively on the generator constructions in Chapter 6. Chapters 7 and 8 are essentially my own work. Throughout the thesis all examples and detailed computations are my work and in particular the extensive application of the CoCoA and Maple packages (with the exception of the programme to compute Gröbner bases over the field of complex numbers that was developed in collaboration with Caboara).

Summary

The thesis is essentially concerned with two subjects corresponding to the two grants under which the author was research assistant in the last three years. The one presented first, which cronologically comes second, addresses the issues of identifiability for polynomial models via algebraic geometry and leads to a deeper understanding of the classical theory. For example the very recent introduction of the idea of the *fan* of an experimental design gives a maximal class of models identifiable with a given design. The second area develops a theory of optimum orthogonal fractions for Fourier regression models based on integer lattice designs. These provide alternatives to product designs. For particular classes of Fourier models with a given number of interactions the focus is on the study of orthogonal designs with attention given to complexity issues as the dimension of the model increases. Thus multivariate identifiability is the field of concern of the thesis. A major link between these two parts is given by Part III where the algebraic approach to identifiability is extended to Fourier models and lattice designs. The approach is algorithmic and algorithms to deal with the various issues are to be found throughout the thesis.

Both the application of algebraic geometry and computer algebra in statistics and the analysis of orthogonal fractions for Fourier models are new and rapidly growing fields. See for example the work by Koval and Schwabe (1997) [42] on qualitative Fourier models, Shi and Fang (1995) [67] on *U*-designs for Fourier regression and Dette and Haller (1997) [25] on one-dimensional incomplete Fourier models. For algebraic geometry in experimental design see Fontana, Pistone and Rogantin (1997) [31] on two-level orthogonal fractions, Caboara and Robbiano (1997) [15] on the inversion problem and Robbiano and Rogantin (1997) [61] on distracted fractions. The only previous extensive application of algebraic geometry in statistics is the work of Diaconis and Sturmfels (1993) [27] on sampling from conditional distributions.

“Lasciate ogne speranza, voi ch'intrate.”

Dante, *Divina Commedia*, Inferno, III-9

Chapter 1

Introduction

In this thesis we present novel techniques based on symbolic computation to study multidimensional identifiability for polynomial and Fourier models. Broadly speaking we look for pairs (Design, Model) such that the usual experimental design matrix is full rank. Within this framework we consider two specific problems which correspond to the first two parts of the thesis. The third part links the previous two. In the first part we consider a design D with N distinct points in the d -dimensional affine space. We use algebraic geometry and specifically Gröbner bases to find a set of N polynomial terms called *Est* such that the design matrix of a model based on *Est* at D is invertible. An identifiable linear model can then be built from *Est*. The use of computer algebra packages is instrumental. We used Maple and CoCoA. The interaction between statistics (identifiability in experimental design) and algebra (Gröbner bases) was beneficial to both. For example on one hand the proper algebraic notion of fan of an ideal led to the definition of maximal fan designs that identify a broader class of models than for example full factorial designs and showed nice similarities with space-filling designs (see Section 3.3). On the other hand the application of algebraic geometry to experimental design has awoken a new interest in zero-dimensional ideals within the algebraic community (see Caboara and Robbiano [15]). The concept of aliasing and confounding classes finds an explicative algebraic counterpart in the definition of the quotient space.

In the second part of the thesis we consider Fourier type regression vectors and lattice designs used in numerical integration and number theory. We tackle both the direct problem and the inverse problem. Given a design D we are able to determine classes of models for which D is orthogonal. Orthogonality implies identifiability and some optimal design criteria such as D -optimality. Moreover by exploiting the group structure of lattice designs the notion of aliasing has been fully explained in this context in terms of the relationship with the so-called dual lattice of the design. We show how a double coset structure generalises the notion of Nyquist folding from Fourier analysis.

As expected, the inverse problem, finding a design with a given property, turns out to be less nicely encoded into the algebra of dual lattices than the direct problem. Nevertheless we have been able to solve it for the most interesting classes of models, that is additive models and two-factor interaction models. We find orthogonal designs exploiting symbolic computation in the form of recurrence generating sequences and an algorithm which has a good implementation in CoCoA. Partic-

ular attention is given to complexity issues as the dimension increases which are essentially generalisations of Nyquist sampling theory to lattices.

In the third part of the thesis we reparametrize Fourier models in polynomial form. After adjoining a set of polynomials encoding the Fourier nature of the problem, namely the fact that $\sin^2 x + \cos^2 x = 1$, we can apply the algebraic-geometric procedure of the first part of the thesis to Fourier models.

Very briefly we can say that in classical experimental design when we plan an experiment one should have a clear idea of what the aim of the experiment is. For example if we want to model some phenomenon then we must have an idea of the model structure expressed as a certain polynomial of certain degree. Then we choose the design sites at which to take observations in such a way as to satisfy various criteria such as complete randomization or D -optimality according to the aim of the experiment (for the equivalence between various optimal criteria see Pukelsheim [54] and Silvey [68]). Alternatively one could fit a model within a class to the given design/observations and analyse the error, for example in prediction. The algebraic procedure we present returns a regression vector which depends only on the design points and the important entity called a term-ordering (and the dependence on the term-ordering can be removed —see the fan of a design, Section 3.3). That is, it depends on the spatial structure of the design and it does not require much a priori knowledge from the experimenter. Of course we are still within a specific class of models (polynomial and Fourier are considered in the thesis) but the large number of term-orderings allows us to span among many model structures.

Next we describe Part I in details. It consists of two chapters. We believe this is a first systematic use of Gröbner bases in Statistics and experimental design. Chapter 2 is a specially written introduction to the theory of Gröbner bases. The ring of multivariate polynomials under the operations of sum and product is described in Section 2.1. In this context the notion of term-ordering occurs naturally (see Subsection 2.1.1). The division of polynomials plays an important role in both the algebraic theory and its application to experimental design and it is described in Subsections 2.1.2 and 2.1.3. The concept of an affine variety as set of zeros of a system of polynomial equations is the subject of Section 2.2. Gröbner bases described in Section 2.3 are useful equivalent representations of a system of polynomial equations depending on the choice of a term-ordering. Their existence and finiteness are proved for example by the Hilbert basis theorem in Subsection 2.1.4 and they can be computed by the Buchberger algorithm of Subsection 2.3.1. The elimination theory in Section 2.4 allows us to compute the Gröbner basis of the projection of the system on a subset of the input variables and in particular to solve the system, if a solution exists. Finally, Section 2.5 describes polynomial functions as the evaluation of polynomials that admit one and only one output for each input in a suitable domain space. Also the quotient by ideals, that plays a key role in the subsequent application, is introduced.

Chapter 3 describes and amplifies the computational algebraic procedure of Pistone and Wynn (1996) [53]. It uses Gröbner bases to solve estimability/identifiability problems in the design of experiments for polynomial models. The methodology is applied to a case study in Holliday, Pistone, Riccomagno and Wynn (1997) [37]. In the thesis every single step of the theory has been checked on the computer for example implementing the various procedures. The idea is to shift the focus from the

design as a set of points to the design variety and its associated polynomial ideal, namely the set of polynomials whose solutions are the design points. Thus each factor of a statistical experiment corresponds to an indeterminate in the algebraic framework, a design corresponds to an ideal, and the mean of a statistical linear additive polynomial model is associated to a polynomial. Given a term-ordering on the indeterminates/factors, Gröbner basis techniques allow us to determine an estimable saturated model, that is a polynomial with as many (estimable) terms as design points. This identifiable model corresponds to the order ideal associated to the Gröbner basis of the design ideal (see Section 3.2). The necessity of a term-ordering which at first seemed a limit to the theory has been overcome in part by the idea of the fan of an experimental design (see Section 3.3 and Caboara, Pistone, Riccomagno and Wynn, 1997 [13]) and in part by a new understanding of the concept of aliasing of models and of terms within a model as equivalence classes modulo the design ideal. In Section 3.4 we extend the notion of design ideal to include observations as parameters when their real values are unknown. All of Chapter 3 is accompanied by examples. Let us be more specific.

The basic observation of Pistone and Wynn (1997) [53] is that a *design* D is a zero-dimensional variety. The ideal associated to the design, $I(D)$ has a nice interpretation in terms of interpolation as the set of all polynomial functions whose zeros include the design points. We review comprehensively and extend the original theory and present some other results.

Let $k[x_1, \dots, x_d]$ be the set of all polynomials in the indeterminates x_1, \dots, x_d and with coefficients in k , where k is a field, typically the set of rational numbers \mathbb{Q} . The elements of $k[x_1, \dots, x_d]$ are referred to as polynomial models. Let $D = \{\mathbf{x}^{(i)} : i = 1, \dots, N\}$ be a finite set of distinct points in k^d . Let τ be a (rational) term-ordering on the set of monomials of $k[x_1, \dots, x_d]$. Often τ will be the *lexicographic ordering* or the *reverse total degree ordering*. Specific characteristics of the actual problem will help in the choice of the term-ordering and in particular the initial ordering on the factors/indeterminates x_1, \dots, x_d .

It turns out that the quotient set $k[x_1, \dots, x_d]/I(D)$ (the set of remainders with respect to the polynomial division) is the set of *models* identifiable by the design D . Operationally we proceed as follows. Let $G = \{g_1, \dots, g_t\}$ be a Gröbner basis for the design ideal $I(D)$ with respect to the term-ordering τ . Then the set of all monomials not divisible by any of the leading terms of the elements of G gives a vector-space basis of $k[x_1, \dots, x_d]/I(D)$. Call it $BG = \{\mathbf{x}^\alpha\}$. The *order ideal* structure of such a basis has a nice interpretation which the theory exploits. Suppose that at each design point $\mathbf{x}^{(i)}$ an observation Y_i is taken. Then any model of the form $\sum_{\mathbf{x}^\alpha \in BG} \theta_\alpha \mathbf{x}^\alpha$ is identifiable in the sense that the θ_α are uniquely determined as solutions of the following system of linear equations: $Y_i = \sum_{\mathbf{x}^\alpha \in BG} \theta_\alpha \mathbf{x}^\alpha(\mathbf{x}^{(i)})$.

Since the dimension as vector-space of $k[x_1, \dots, x_d]/I(D)$ equals the number of design points (whatever term-ordering one chooses) we have that the saturated model estimable by a design with N elements has exactly N terms. This was a subliminal even if unstated fact in experimental design.

In this algebraic formulation the confounding/aliasing question is posed and answered in the following terms. We discuss this at length in Section 3.2. Two polynomial models f and g are confounded under the design D and with respect to the ordering τ if and only if $Rem(f, G) = Rem(g, G)$, where the operator Rem returns nor-

mal forms with respect to G . Then we have $Y_i = f(\mathbf{x}^{(i)}) = \text{Rem}(f, G)(\mathbf{x}^{(i)}) = g(\mathbf{x}^{(i)})$ for all design points $\mathbf{x}^{(i)}$. In particular let us decompose any polynomial f into a leading term $Lt(f)$ and a tail $t(f) := Lt(f) - f$. If G is a reduced Gröbner basis then for all $g \in G$ we have that $Lt(g)$ is confounded with $t(f)$. This can be seen as the counterpart of the aliasing tables in experimental design.

In Part II of the thesis we present a theory of orthogonal experimental fractions for complete Fourier regression models (that uses one-generator integer lattice designs) started in Riccomagno, Schwabe and Wynn (1997) [58]. The work is mainly concerned with complexity issues as the dimension increases. The idea was introduced with an example in Bates, Buck, Riccomagno and Wynn (1995) [3] and the orthogonality conditions are expressed in terms of group theory in Bates, Riccomagno, Schwabe and Wynn (1995) [4].

In Chapter 4 we define and give examples of Fourier models (Section 4.1) and lattice designs (Section 4.3) with a particular mention of multirank lattice designs in Subsection 4.3.1. In Subsection 4.3.2 there is a basic formula to compute the error of a quadrature formula based on lattice grids on which we base the theory of orthogonal designs for Fourier regression of Chapter 5.

Chapter 5 is divided into six sections. The first two are introductory examples to the general theory of one-generator lattice designs for Fourier models that are presented in Sections 5.4 and 5.5. The proofs of Section 5.3 follow immediately from the general theory and the section has been reversed in the exposition for clarity. Finally in Section 5.6 the theory is extended to multirank lattice designs.

Chapter 6 deals with the inverse problem for complete Fourier models. Good generators are sought in the class of one-generator lattices for which the sample size is generally smaller than the sample size of multi-rank lattices. In particular we study additive models and two-factor interaction models in Sections 6.3 and 6.4 respectively for which the difference between number of parameters and sample size of a product design is bigger. These sections are accompanied by a series of figures and tables which describe and compare the behavior of lattice designs chosen within a given class. Comparison are made between various kinds of lattice designs and preference is given to designs with sample sizes increasing polynomially with the dimension of the model. The various kinds of designs are described in Section 6.1 and in Section 6.2 we give rules to compute suitable sample sizes.

In the last chapter of Part II we show how one-generator lattice designs can be used for fast detection of important factors in a high dimensional model by tricking the model into a one-dimensional structure and exploiting the properties of the one-dimensional Fourier transform. Section 7.2 computes the error when observations are taken without error from a known function at a given lattice design and it is subject to further study. More theory follows.

Bates, Buck, Riccomagno and Wynn (1996) [4] mention that integer lattice designs are D -optimum in the sense of Kiefer and Wolfowitz (1959) [40] 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

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

$x \in [0, 1)$, 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 normalising factor $\sqrt{2}$ is included in the model equation 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.

We introduce the notation $F(d; m_1, \dots, m_d; M)$ for the complete Fourier model in d dimensions with one-dimensional “marginal” models for x_1 to x_d respectively of orders m_1 to m_d and in which all interactions up to M factors are included.

Integer lattices have been used extensively in numerical integration. The books by Niederreiter (1992) [50], Conway and Sloane (1992) [22], Sloan and Joe (1994) [69] and Fang and Wang (1994) [29] are basic references. Periodic and indeed Fourier models are the natural models to be associated with the methods because of the periodic nature of the lattices themselves. In this thesis we investigate lattices as experimental designs for fitting Fourier models. It will be seen that as with classical polynomial models orthogonality plays an important role and yields D -optimum designs (Kiefer and Wolfowitz, 1959 [40]). Orthogonality will be related to the so-called “dual lattice” and there is a strong connection with classical designs based on defining subgroups and aliasing.

The challenge of the theory, as we see it, is to solve “inversion” problems. That is, given a particular model find the lattice which as an experimental design allows us orthogonal estimation of all terms in the model, without aliasing. In this respect the thesis continues the work in Riccomagno, Schwabe and Wynn (1997) [58].

Models built on space filling designs are becoming popular in building emulators, or surrogates, of large and expensive-to-run simulation codes in computer aided design and similar areas. This body of research started with the work by Sacks, Welch, Mitchell and Wynn (1989) [62]. A restriction of the Fourier models is the assumption of periodicity. One can try to avoid this restriction by enlarging, shifting, or randomising the start of the design. Also there are methods for periodising non-periodic functions, see Sloan and Joe (1994) [69]. The author’s and coauthors’ preliminary conclusions from the practical use of these methods is that they are valuable, at least, for *screening*, that is detection of significant factors very much in the style of screening designs based on orthogonal arrays which have become popular in “Taguchi” methodology in Robust Engineering Design (see Section 7.1).

A major purpose for this thesis is to show how to base observations on lattices reduces the complexity of fitting Fourier models. If not all interactions (cross spectral) terms are fitted then the number of observations required for orthogonality may be linear or polynomial in the dimension rather than exponential. Thus the work can be seen as presenting a type of computational complexity result. From the point of view of Fourier analysis, for example of the kind used in signal processing, the work

can be considered as introducing a special kind of Nyquist-Shannon sampling theory based on lattices. It is in such a theory that a trade-off between sampling “rates” and model order is studied.

In the algebraic approach to identifiability of Part I instead of polynomial models one can consider some other classes of models. In particular Part III analyses Fourier models of the kind $\sum_{j=1}^v \theta_j \sin(2\pi\alpha_j^t x) + \phi_j \cos(2\pi\beta_j^t x)$. Roughly speaking two indeterminates c_k and s_k are associated to each factor x_k . In this way a one-to-one correspondence is created between the class of Fourier models, \mathcal{F} and the polynomial ring $\mathcal{M} := k[c_1, \dots, c_d, s_1, \dots, s_d]/(c_k^2 + s_k^2 - 1 : k = 1, \dots, d)$. Now the algebraic procedure can be applied in \mathcal{M} and the output translated back to \mathcal{F} . Care should be taken in the interpretation of the results. (A paper on this subject in collaboration with Caboara, who carried out most of the computational aspects of simple algebraic extension of rational fields, is under revision for publication on the *Journal of Symbolic Computation*).

The appendices give a summary of a considerable volume of computational algebra work which formed an integral part of the thesis and the joint research programme of which it is a part.

Part I

**Gröbner Bases in Experimental
Design**

Chapter 2

Introduction to Gröbner bases

In this chapter we introduce the tools of algebraic-geometry theory that we use in the thesis. Our presentation covers the algebraic-geometry concepts and other matters of relevance for applications and their statistical counterparts. We only describe material specifically relevant while endeavouring to be mathematically precise. The interested reader is referred to the specialised texts in the bibliography for example Cox, Little and O'Shea (1992) [24], Adams and Loustau (1994) [1] and Mora (1994) [47]. Gröbner bases were introduced by B. Buchberger (1965) and became a powerful tool in many fields, [2, 6, 30, 35, 38, 70, 72].

2.1 Polynomials and polynomial ideals

We work in the space $k[x_1, \dots, x_d]$, the commutative ring of all polynomials in the indeterminates x_1, \dots, x_d and with coefficients in k , where k is a field. Most of the time k will be the rational numbers, \mathbb{Q} . The elements of $k[x_1, \dots, x_d]$ of the form $\alpha x_1^{\alpha_1} \dots x_d^{\alpha_d}$ with $\alpha_i \in \mathbb{Z}_+$ for all $i = 1, \dots, d$ and $\alpha \in k$ are called monomials or, when $\alpha = 1$, terms. The set of all terms in $k[x_1, \dots, x_d]$ is denoted by T^d . A polynomial is a k -linear combination of terms.

Definition 1 *A model is an element of $k[x_1, \dots, x_d]$ or a finite subset of $k[x_1, \dots, x_d]$.*

Examples of models are (i) $1 + x_1 + x_2 + x_1x_2 \in \mathbb{Q}[x_1, x_2]$ where the coefficients assume rational values; (ii) the one dimensional quadratic model, $\theta_0 + \theta_1x_1 + \theta_2x_1^2 \in \mathbb{Q}(\theta_0, \theta_1, \theta_2)[x_1]$ where $k = \mathbb{Q}(\theta_0, \theta_1, \theta_2)$ is the field of polynomial fractions in the parameters $\theta_0, \theta_1, \theta_2$ and with rational coefficients; (iii) the model $x_1^2 + x_2^2 \in \mathbb{Z}_3[x_1, x_2]$ where the coefficient field is finite; (iv) the model $\{\theta_2x_1^2 + \theta_1x_2^2 - \theta_0, x_1x_2 - 1\}$ in $\mathbb{Q}(\theta_0, \theta_1, \theta_2)[x_1, x_2]$ which may be considered as the model $\theta_2x_1^2 + \theta_1x_2^2 - \theta_0$ subject to the constraint $x_1x_2 - 1 = 0$.

To help the notation, we often denote x_1, \dots, x_d as \mathbf{x} . Also sometimes we use x, y, z instead of x_1, x_2, x_3 .

Most of the time we shall consider a polynomial $f \in k[\mathbf{x}]$ as the deterministic part of a statistical regression model Y

$$Y(\mathbf{x}) = f(\mathbf{x}) + \epsilon(\mathbf{x})$$

where $\epsilon(\mathbf{x})$ is an error for all \mathbf{x} in a (design) region \mathcal{X} and f is an analytic polynomial function over \mathcal{X} with coefficients in k or $k(\theta_1, \dots, \theta_p)$. It follows that strictly speaking we should distinguish between x_i ($i = 1, \dots, d$) as indeterminate, in particular as $x_i \in k[\mathbf{x}]$ and as analytic variable (statistical factor), in particular as function assuming values over $\mathcal{X} \subset k^d$. This same observation applies to f as a formal polynomial in $k[\mathbf{x}]$ and as an analytic function from \mathcal{X} to k . Understanding the context makes clear whether we are considering formal entities and we shall not overload the text with further mention of these distinctions.

Models other than polynomial statistical models can be posed in this framework, see for example the Fourier model at Chapter 8.

We mostly work over the field of the rational numbers. Indeed for the application of the algebraic theory to classical polynomial regression models the use of rational quantities is not a restriction since in real experiments rational numbers are good approximations to irrational ones.

Sometimes our examples will be over the set of integer numbers, \mathbb{Z} which is not a field. Gröbner basis theory has a counterpart for rings over integer coefficients but there is the problem that *G-basis-related computations could not terminate or be wrong* as CoCoA warns when one inputs the ring $\mathbb{Z}[x_1, x_2]$. However \mathbb{Z} is embedded in \mathbb{Q} and one can work with rational coefficients and multiply everything out to obtain integers. On other occasions one has to work with a finite set of coefficients say \mathbb{Z}_p . When p is a prime integer then \mathbb{Z}_p is a field and the algebraic theory is similar to the one over rational numbers. In other cases, such as the trigonometric case, things are made difficult by the fact that the sine and cosine of rational values are typically irrational numbers and thus the coefficient field is not embeddable in \mathbb{Q} . Ad hoc procedures have been considered based on simple algebraic extensions of rational numbers and we shall discuss them in Chapter 8.

A basic tool is the algebraic structure called an ideal.

Definition 2 *A (polynomial) ideal I is a subset of $k[\mathbf{x}]$ closed under sum and product of elements of $k[\mathbf{x}]$. Specifically the set $I \subset k[\mathbf{x}]$ is an ideal if for all $f, g \in I$ and $h \in k[\mathbf{x}]$ the polynomials $f + g$ and hf are in I .*

Definition 3 *An ideal, I is radical if $f \in I$ whenever a positive integer m exists such that $f^m \in I$.*

Definition 4 *The radical of an ideal is the radical ideal defined as*

$$\sqrt{I} = \{f \in k[x_1, \dots, x_d] : \text{a positive integer } m \text{ exists: } f^m \in I\}.$$

A more practical definition of an ideal than Definition 2 is implicit in Definition 5. The Hilbert basis theorem (see Section 2.1.4) will prove the two definitions equivalent.

Definition 5 *An ideal I is finitely generated if there exist $f_1, \dots, f_s \in k[\mathbf{x}]$ such that $I = \langle f_1, \dots, f_s \rangle$. Specifically for any $f \in I$ there exist h_1, \dots, h_s polynomials of $k[\mathbf{x}]$ such that*

$$f = \sum_{i=1}^s h_i f_i.$$

The set $\{f_1, \dots, f_s\}$ is called a basis of I .

We shall call $f = \sum_{i=1}^s h_i f_i$ a polynomial combination by analogy with linear combinations of vector spaces. In contrast to vector spaces where the elements of a basis must span and be linearly independent over k , an ideal basis needs only to span. This lack of independence, due to the fact that the coefficients are polynomials, is the cause of the difficulty in extending the division algorithm to more than one dimension. It implies that a polynomial in an ideal may be expressed as polynomial combination of the basis elements in different ways. For example in $I = \langle x, y \rangle \subset k[x, y]$ the polynomial $f = 0$ can be expressed both as $f = 0 \cdot x + 0 \cdot y$ and $f = y \cdot x - x \cdot y$. Note that $\{x, y\}$ is a *minimal* basis for I , that is none of its proper subsets is a basis for I . Minimal bases of the same ideal can consist of different number of elements. For example we have $\langle x^2, x + x^2 \rangle = \langle x \rangle$ and both are minimal.

We remark that in one variable there is a privileged generator of an ideal $\langle f_1(x), \dots, f_v(x) \rangle$ namely the greatest common divisor or GCD of f_1, \dots, f_v .

A key point is that the statistical counterpart of an ideal is a design, usually a finite set of points in \mathcal{X} . That is, the set of all polynomial functions whose zeros include the design points is an ideal. This ideal corresponds to an ideal in $k[\mathbf{x}]$: the design ideal. In Section 2.2 we shall reintroduce design ideals through the geometric notion of variety and its well-exploited link to polynomial ideal theory. It may be seen that radical ideals correspond to pointwise designs without replications.

While working with ideals and polynomials some questions arise: (i) how can we characterise an ideal (ideal description)? (ii) When does a polynomial belong to an ideal (ideal membership)? (iii) What links polynomial ideals to system of polynomial equations and their solutions? (iv) What does division mean in more than one variable? The statistical counterparts of these questions are (i) how to characterise designs? (ii) What is a minimal number of polynomials to define a design? (iii) How is this related to more familiar issues such as interpolation and confounding?

2.1.1 Orderings

Throughout this thesis we follow the standard notation as in Cox, Little and O'Shea (1992) [24]. For example $I = \langle f : f \in A \rangle$ is the ideal generated by the elements of $A \in k[\mathbf{x}]$, equivalently the elements of A form a basis for I .

Definition 6 We order the indeterminates (or factors) x_1, \dots, x_d by an initial ordering, for example $x_d < \dots < x_2 < x_1$.

Specific knowledge of the problem intervenes in the choice of the initial ordering (and of the ordering in general). In Section 3.3 we see how the special idea of fan of ideals allows us to drop the assumption of having an a-priori initial ordering (and in general a term ordering).

A one-to-one correspondence between monomials of $k[x_1, \dots, x_d]$ and the d -dimensional vectors with non-negative integer components is widely used. For example in $k[x_1, x_2, x_3]$ with $x_3 < x_2 < x_1$ the monomial $x_1^7 x_3^2$ corresponds to the vectors $[7, 0, 2]$ and x_1 to $[1, 0, 0]$. This correspondence is referred to as multi-index representation of monomials or *log function*. Thus $\mathbf{x}^\alpha = x_1^{\alpha_1} \dots x_n^{\alpha_n}$ goes into $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{Z}_+^d$ with the convention that $x_n < x_{n-1} < \dots < x_2 < x_1$.

Definition 7 A monomial or term ordering on $k[\mathbf{x}]$ is a totally ordering relation $<$ (or τ) on T^d , that is the terms of $k[\mathbf{x}]$, satisfying

1. $1 < \mathbf{x}^\alpha$ for all \mathbf{x}^α with $\alpha \neq 0$ and
2. for all α, β, γ such that $\mathbf{x}^\alpha < \mathbf{x}^\beta$, then $\mathbf{x}^\alpha \mathbf{x}^\gamma < \mathbf{x}^\beta \mathbf{x}^\gamma$

where $\alpha, \beta, \gamma \in \mathbb{Z}_+^d$ and $\mathbf{x} = (x_1, \dots, x_d)$.

When it is needed to indicate the initial ordering of the term ordering τ we write $\tau(x_n < \dots < x_1)$. Definition 7 implies the following three facts. (i) Any two monomials are comparable, that is for any $\mathbf{x}^\alpha, \mathbf{x}^\beta$ either $\mathbf{x}^\alpha < \mathbf{x}^\beta$ or $\mathbf{x}^\alpha = \mathbf{x}^\beta$ or $\mathbf{x}^\beta < \mathbf{x}^\alpha$. This property characterises total orderings. (ii) There is no infinite descending chain. In particular any subset of monomials contains a minimum element with respect to the ordering. This property is known as well-ordering. (iii) The ordering is compatible with the multiplication, that is for any pair of polynomials \mathbf{x}^α and \mathbf{x}^β , if \mathbf{x}^α divides \mathbf{x}^β then $\mathbf{x}^\alpha < \mathbf{x}^\beta$.

Let us prove Point (iii). Since \mathbf{x}^α divides \mathbf{x}^β there exists \mathbf{x}^γ greater or equal to 1 such that $\mathbf{x}^\beta = \mathbf{x}^\alpha \mathbf{x}^\gamma$. Thus we conclude either $\mathbf{x}^\beta = \mathbf{x}^\alpha \mathbf{x}^\gamma > \mathbf{x}^\alpha 1$ or $\mathbf{x}^\beta = \mathbf{x}^\alpha \mathbf{x}^\gamma = \mathbf{x}^\alpha 1$.

Referring to the multi-index notation and fixed an initial ordering, the term orderings mostly used in applications are the lexicographic ordering and the total degree reverse lexicographic ordering defined as follows.

- lex:** $\mathbf{x}^\alpha >_{lex} \mathbf{x}^\beta$ equivalently $\alpha >_{lex} \beta$ if and only if the left-most nonzero entry of $\alpha - \beta$ is positive. In this ordering a variable dominates the monomials regardless of the degree of the other variables. This ordering is also called **plex**.
- tdex:** $\alpha >_{tdex} \beta$ if and only if $\sum_{i=1}^d \alpha_i > \sum_{i=1}^d \beta_i$ or $\sum_{i=1}^d \alpha_i = \sum_{i=1}^d \beta_i$ and $\alpha >_{invlex} \beta$ that is the right-most nonzero entry of $\alpha - \beta$ is negative. This ordering first takes in account the total degree of monomials and then orders in an inverse lexicographical way. This ordering is also called **degrevlex**.

Definition 8 Let τ be a term ordering on $k[\mathbf{x}]$. The leading term of f , $Lt_\tau(f)$ is the greatest term with respect to τ among the terms in f . The leading coefficient, $Lc_\tau(f)$ is the coefficient of $Lt_\tau(f)$. The leading monomial, $Lm_\tau(f)$ is the product $Lc_\tau(f)Lt_\tau(f)$.

Most of the time we drop the suffix τ . For $Q[x, y, z]$ with **degrevlex** ($z < x < y$) we have $Lt(3xy^2z + \frac{1}{2}xyz^2 + 3x^2) = xy^2z$ and for $Q[x, y, z]$ with **lex** ($z < y < x$) $Lt(3xy^2z + \frac{1}{2}xyz^2 + 3x^2) = x^2$. In both cases the leading coefficient is 3.

Some computer packages such as CoCoA and Macaulay allow the user to define custom-built orderings, using the fact that each ordering corresponds to a (non unique) array U of integer vectors with the first non-zero element in each column positive and then $\alpha >_U \beta$ if and only if $\alpha U >_{lex} \beta U$. We develop this in more detail before listing some orderings and corresponding matrices. The reader is referred to Mora and Robbiano, 1988 [49] and Adams and Loustau (1994) [1] pp. 166ss.

The orderings on $k[\mathbf{x}]$ compatible with the ring operations are classified in Robbiano (1985) [60]. We here briefly sketch such classification for rational term-orderings, the only ones of interest for this work. A matrix $M(\tau) \in M_{d \times d}(\mathbb{Q})$ is

associated to an ordering τ over $k[x_1, \dots, x_d]$. If the matrix $M(\tau)$ has full rank, then τ is a total ordering. A total rational orderings τ is such that

$$t >_{\tau} 1 \forall t \in T^d \Leftrightarrow \text{for every column of } M(\tau) \text{ the first non null entry is positive.}$$

The ordering τ is built from $M(\tau)$ using the natural multi-index bijection

$$\begin{aligned} \log : \quad T^d &\longrightarrow \mathbb{Z}_+^d \\ \mathbf{x} = (x_1^{\alpha_1} \dots x_d^{\alpha_d}) &\longmapsto (\alpha_1, \dots, \alpha_d) \end{aligned}$$

defining τ by

$$\mathbf{x} >_{\tau} \mathbf{x}' \Leftrightarrow \text{the first non null component of } M(\tau) \cdot (\log(\mathbf{x}) - \log(\mathbf{x}')) \text{ is positive}$$

which is if and only if

$$\mathbf{x}^{M(\tau) \cdot \log(\mathbf{x})} <_{\text{lex}} \mathbf{x}'^{M(\tau) \cdot \log(\mathbf{x}')}.$$

We could also say if and only if

$$M(\tau) \cdot \log(\mathbf{x}) <_{\text{lex}} M(\tau) \cdot \log(\mathbf{x}')$$

referring to the lexicographic ordering over \mathbb{Z}_+^d .

The **lex** term ordering is associated to the identity matrix. In $\mathbb{Q}[x_1, x_2, x_3]$ we have

$$M(\text{lex}) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

that is

$$\mathbf{x} > \mathbf{x}' \Leftrightarrow \text{deg}_{x_1}(\mathbf{x}) > \text{deg}_{x_1}(\mathbf{x}') \text{ or } \text{deg}_{x_1}(\mathbf{x}) = \text{deg}_{x_1}(\mathbf{x}') \text{ and } \text{deg}_{x_2}(\mathbf{x}) > \text{deg}_{x_2}(\mathbf{x}').$$

For example $x_1^2 x_2^5 > x_1 x_2^{12}$, $x_1^2 x_2^2 > x_1^2 x_2$.

In $\mathbb{Q}[x_1, x_2, x_3]$, the term-ordering associated with the matrix

$$M(\tau) = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$$

is the **tddeg** term-ordering that is the ordering for which

$$\mathbf{x} > \mathbf{x}' \Leftrightarrow \begin{cases} \text{deg}(\mathbf{x}) > \text{deg}(\mathbf{x}') \\ \text{or} \\ \text{deg}(\mathbf{x}) = \text{deg}(\mathbf{x}') \text{ and the last non zero entry} \\ \text{in } (\log(\mathbf{x}) - \log(\mathbf{x}')) \text{ is } < 0. \end{cases}$$

For the **tddeg** term-ordering, $x_1 x_2^5 > x_1^2 x_2^3$, $x_1^2 x_2^2 > x_1^2 x_2$. Notice how these definitions are consistent with the ones given before.

If the first row of the matrix associated to the term-ordering τ is the vector $(1, \dots, 1)$, then τ is a degree-compatible term-ordering, that is it takes into account the total degree of terms. Notice that because of the matrix U ordering monomials reduces to a collection of inequalities.

The knowledge one has on the interdependencies of the variables of a real problem is usually not total but only partial. A Gröbner basis theory has been developed for partial orderings. A complication is that the algorithm for computation of Gröbner bases usually does not terminate. A solution is to pack the partial ordering into a total term ordering by choosing arbitrarily a leading term in case of equality in the partial ordering. This leads to the notion of the *fan* of an ideal in Section 3.3. A fan gives all the possible Gröbner bases of an ideal, and importantly there are a finite number of them. The fan of an ideal generates the equivalence classes of term orderings modulo the ideal.

2.1.2 Division

The operations over $k[x]$ we mostly use are (i) sum, corresponding for example to sum of models, (ii) product with scalar, corresponding for example to scaling of models, (iii) product of polynomials, useful in the definition of design ideals and (iv) polynomial division, in particular simplification of monomial fractions.

The first three operations are natural while the polynomial division needs to be discussed and it requires the notion of term ordering. For univariate polynomial division and division algorithm are well-known and summarised in the following theorem.

Theorem 1 *For every $f, g \in k[x]$ there exist unique $s_g, r \in k[x]$ such that $\deg(r) < \deg(g)$ and $f = s_g g + r$, where $\deg(f)$ is the degree of f . The division algorithm returns s_g and r .*

In more than one dimension things are different.

Theorem 2 *Let f, g_1, \dots, g_t be in $k[x]$. It still holds that the division of f by g_1, \dots, g_t gives a decomposition of f on g_1, \dots, g_t in the sense that there exist $s_1, \dots, s_t \in k[x]$ and $r \in k[x]$ such that*

$$f = \sum_{i=1}^t s_i g_i + r$$

and r is not divisible by any of the $Lt_\tau(g_i)$ for $i = 1, \dots, t$ where τ is a given term ordering.

Definition 9 *The polynomial r of the previous two theorems is called the remainder. Sometimes instead of r we write $\text{Rem}(f, g)$ and $\text{Rem}(f, \{g_1, \dots, g_t\})$ or $\text{Rem}(f, G)$ where $G = \{g_1, \dots, g_t\}$.*

Unfortunately the division is not a proper operation over the polynomial ring since in general its output is not unique as the following example shows

$$x^2y + xy^2 + y^2 = (x + 1)(y^2 - 1) + x(xy - 1) + 2x + 1$$

if we divide first by $y^2 - 1$ and

$$x^2y + xy^2 + y^2 = (x + y)(xy - 1) + (y^2 - 1) + x + y + 1$$

if we divide first by $xy - 1$. This has consequences in interpolation: for any finite set of points in \mathbb{R}^d ($d > 1$) there is more than one interpolating polynomial. This poverty of the division algorithm is overcome by choosing a term ordering and using Gröbner bases, effectively by expressing a preference over which terms should appear in the interpolator.

The division in one-dimension allows us to solve the ideal membership problem: a one-dimensional polynomial f belongs to the ideal generated by $g \in k[x]$ if and only if $Rem(f, g) = 0$. We shall see that in higher dimension a polynomial belongs to an ideal if and only if the remainder of the polynomial with respect to a Gröbner basis of the ideal is zero.

The ideal description problem, that is the problem of finding a finite set of generators, is solved for one-dimensional ideals by the Euclidean algorithm: a basis for the ideal generated by f_1, \dots, f_n is the greatest common divisor of f_1, \dots, f_n . In more than one-dimension and given a term ordering an ideal is uniquely described by its reduced Gröbner basis (see Section 2.3).

2.1.3 Division algorithm

At each step of the division algorithm in one-dimension the term of maximum degree (the leading term) of the dividend is well defined and it is divided by the leading term of the divisor.

The notion of term ordering makes possible the division algorithm for multidimensional polynomials by allowing us to select leading terms. The simplification of monomials as known from elementary algebra is the foundation of the division algorithm. Thus we recall that \mathbf{x}^α divides \mathbf{x}^β if and only if all the components of $\alpha - \beta$ are greater or equal to 0. We have already used monomial simplification after Definition 7 where it is justified by Item 2 of the definition itself.

Let us show how the division algorithm works via an example. In $Q[x, y, z]$ with the degrevlex($x > y > z$) ordering we want to divide $x^3zy^2 + y$ by $xy + z, xz$ and z in the giving sequence. The scheme goes as follows

$$\begin{array}{l}
 s_1 : x^2zy - xz^2 \\
 s_2 : z^2 \\
 s_3 : \\
 \begin{array}{l|l}
 g_1 : xy + z & x^3zy^2 + y \\
 g_2 : xz & x^3zy^2 + z^2x^2y \\
 g_3 : z & \hline
 & -x^2z^2y + y \\
 & -x^2z^2y - xz^3 \\
 & \hline
 & -xz^3 + y \\
 & -xz^3 \\
 & \hline
 & y
 \end{array}
 \end{array}$$

First we notice that $Lt(x^3zy^2 + y)$ is divided by $Lt(xy + z)$ giving x^2zy . We multiply it by $xy + z$ and subtract from $x^3zy^2 + y$ getting $x^3zy^2 + y = (xy + z)x^2zy + (-x^2yz^2 + y)$. Again $Lt(-x^2yz^2 + y)$ is divided by $Lt(xy + z)$ and we have $x^3zy^2 + y = (xy + z)(x^2zy - xz^2) + (xz^3 + y)$. Now $Lt(xz^3 + y)$ is not divisible by $Lt(xy + z)$ but by $Lt(xz)$ and we have $x^3zy^2 + y = (xy + z)(x^2zy - xz^2) + (xz)(z^2) + (1)(y)$. Since $Lt(y)$ is not divisible by any of $Lt(xy + z)$, $Lt(xz)$ and $Lt(z)$, y is the remainder of

the division.

Remember that the division is not a proper operation since its result, and thus the output of the above algorithm, depends on which order the dividends g_1, \dots, g_t are considered. Gröbner basis theory addresses this issue. The division algorithm is discussed in much literature, in Table 2.1 we report the code from Cox, Little and O'Shea (1992) [24].

2.1.4 Hilbert basis theorem

It is now useful to define *monomial ideals* which are important in the definition of Gröbner basis, and *Dickson's Lemma*, which solves the ideal description and ideal membership problems for monomial ideals. Its analogue for polynomials is the Hilbert basis theorem.

Definition 10 *A monomial ideal is an ideal I of $k[x]$ generated by a (possibly infinite) set of monomials, in the multindex notation*

$$I = \langle x^\alpha : \alpha \in A \subset \mathbb{Z}_+^d \rangle.$$

The set generated by the leading terms of an ideal is an example of monomial ideal and we write $\langle Lt(I) \rangle = \langle Lt(f) : f \in I \rangle$. As another example consider $I = \langle x^4y^6, x^5y^5, x^6 \rangle$. Every term of any element of I is a k -linear combination of the monomials in the right side of the *leading edge* in Figure 2.1.

We outline here the idea of projection. The projections of the ideal I with respect to, say, x_i and x_j is the ideal $I \cap k[x_i, x_j]$, that is: set to zero all the variables but x_i and x_j . In particular $I_p = I \cap k[x_{p+1}, \dots, x_n]$ is called the p -th elimination ideal of I and is extensively used in *elimination theory* (see Section 2.4), for example to triangularise a system of polynomial equations.

Theorem 3 (Dickson's Lemma) *Every monomial ideal has a finite basis of monomials.*

Proof. Let a term ordering on $k[x_1, \dots, x_d]$ be fixed. The proof proceeds by induction on the number of variables and is constructive. Let $I = \langle x^\alpha : \alpha \in A \subset \mathbb{Z}_+^d \rangle$ be the ideal. If $d = 1$ then I is generated by $\min_{\alpha \in A} x_1^\alpha$. The minimum exists as the term ordering is well-ordered. By inductive hypothesis let assume that the theorem is true for $d - 1$. Then rename the last variable in $k[x_1, \dots, x_d]$ that is $x_d = y$ and define the monomial ideal J such that

$$k[x_1, \dots, x_{d-1}] \cap J = \{x^\alpha \in k[x_1, \dots, x_{d-1}] : \text{there exists } m \text{ s.t. } x^\alpha y^m \in I\}.$$

The ideal J can be seen as the restriction of I into $k[x_1, \dots, x_{d-1}]$. By inductive hypothesis we have

$$J = \langle x^{\alpha_1}, \dots, x^{\alpha_{d-1}} \rangle.$$

By definition of J for each α_i there exists m_i such that $x^{\alpha_i} y^{m_i} \in I$. Let m be the maximum of these m_i 's. Then for each $k = 0, \dots, m - 1$ define

$$k[x_1, \dots, x_{d-1}] \cap J_k = \langle x^\beta : x^\beta y^k \in I \rangle = \langle x^{\alpha_{k1}}, \dots, x^{\alpha_{ksk}} \rangle.$$

Input	$G = (g_1, \dots, g_t)$ and f	
Output	$S = (s_1, \dots, s_t)$ and r	such that $f = \sum_{i=1}^t s_i g_i + r$ and $Lt(r)$ is not divisible by $Lt(g_i)$ and $r := 0$
$g_1 := 0$	$g_1 = g_2 \dots = g_t$	
$p := f$		
WHILE	$p \neq 0$ DO	
	$i := 1$	
	divisionoccured:=0	
	WHILE $i \leq t$ AND	divisionoccured = FALSE DO
		IF $Lt(g_i)$ divides $Lt(p)$ THEN
		ELSE
		$g_i := g_i + Lt(p)/Lt(g_i)$
		$p := p - Lt(p)/Lt(g_i)g_i$
		divisionoccured:=true
		$i := i + 1$
	IF divisionoccured	= FALSE THEN
		$r := r + Lt(p)$
		$p := p - Lt(p)$

Table 2.1: Division algorithm.

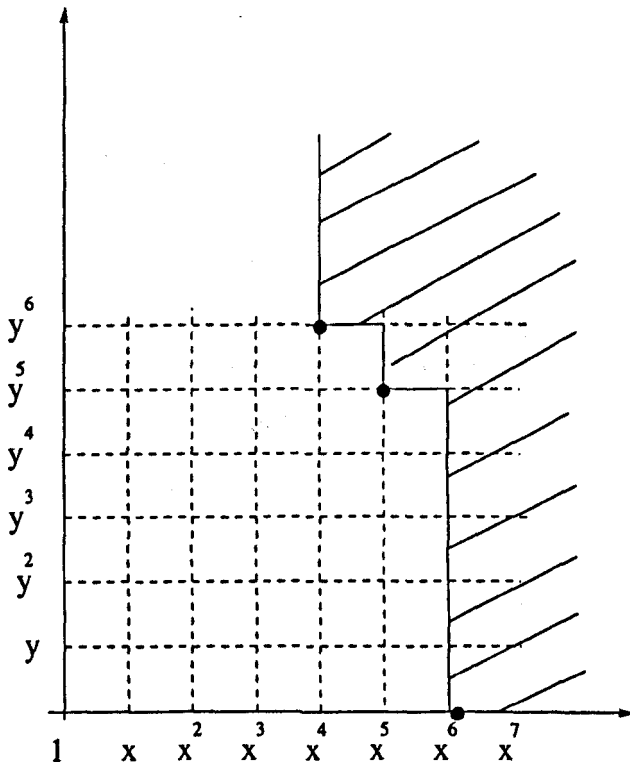


Figure 2.1: Example of order ideal.

Finally I is generated by the following finite list of monomials

$$\begin{aligned} \text{from } J & : x^{\alpha_1}, \dots, x^{\alpha_{n-1}} \\ \text{from } J_0 & : x^{\alpha_{01}}, \dots, x^{\alpha_{0s_0}} \\ \text{from } J_1 & : x^{\alpha_{11}}, \dots, x^{\alpha_{1s_1}} \\ & \vdots \\ \text{from } J_{m-1} & : x^{\alpha_{(m-1)1}}, \dots, x^{\alpha_{(m-1)s_{(m-1)}}}. \end{aligned}$$

Given the arbitrariness of the term ordering we need the proof that such a list generates I , for which we refer to Cox, Little and O'Shea (1992) [24]. ■

A very important consequence of the Dickson's Lemma is its extension to polynomial ideals known as the Hilbert basis theorem.

Theorem 4 (Hilbert Basis Theorem) *Every ideal in $k[x_1, \dots, x_d]$ has a finite basis.*

Proof. Let a term ordering on $k[x]$ be fixed. The set $\langle Lt(I) \rangle = \langle Lt(g) : g \in I \rangle$ is a monomial ideal. The Dickson's lemma states that there exist s polynomials $g_1, \dots, g_s \in I$ such that the ideal generated by their leading terms is the ideal generated by the leading terms of I , that is $\langle Lt(I) \rangle = \langle Lt(g_1), \dots, Lt(g_s) \rangle$.

We want to prove that $\langle g_1, \dots, g_s \rangle = I$. Clearly $\langle g_1, \dots, g_s \rangle \supseteq I$. We prove the converse by contradiction. Let $f \in I$ then from the division algorithm f can be written as $f = \sum_{i=1}^s \alpha_i g_i + r$ where r is not divisible by any of $Lt(g_i)$, $i = 1, \dots, s$. But also $r = f - \sum_{i=1}^s \alpha_i g_i \in I$ thus $Lt(r) \in \langle Lt(g_1), \dots, Lt(g_s) \rangle$, which is a contradiction. ■

We anticipate that the basis given in the proof of Theorem 4 is a Gröbner basis.

2.2 Varieties

Varieties are geometric objects corresponding to polynomial ideals. A system of polynomial equations can be associated to a variety and a variety to an ideal. The link is so strict that many problems arising in the context of varieties can be solved using ideal theory, in particular Gröbner bases, and vice versa.

An *affine variety*, or simply variety, is defined as the affine set of solutions of a system of polynomial equations.

Definition 11 *The variety generated by f_1, \dots, f_s polynomials in $k[x_1, \dots, x_d]$ is*

$$V(f_1, \dots, f_s) = \{(a_1, \dots, a_d) \in k^d : f_h(a_1, \dots, a_d) = 0 \text{ for all } h = 1, \dots, s\}.$$

Definition 12 *Clearly any other polynomial in the ideal generated by f_1, \dots, f_s vanishes on the elements of V . We then talk of the ideal generated by the variety V , the ideal of V , as*

$$I(V) = \{f \in k[x_1, \dots, x_d] : f(a_1, \dots, a_d) = 0 \text{ for all } (a_1, \dots, a_d) \in V\}.$$

The ideal generated by a variety is radical since the square-free decomposition of every polynomial of I is still in I . A polynomial $f \in k[x_1, \dots, x_d]$ is square-free when

in the unique factorisation of f into irreducible polynomials, there are no repeated factors. For example the square-free decomposition of $f = (x^2 - 2)^3(x - 1)(x^3 - 7)^2$ in $\mathbb{Q}[x]$ is $(x^2 - 2)(x - 1)(x^3 - 7)$.

The set $I(\mathbf{V})$ is the set of polynomials interpolating the points in \mathbf{V} . To select one of these polynomials of minimum (in some sense) degree we need a term ordering. The choice of a term ordering is a major point in multi-dimensional interpolation. There are many one-dimensional curves through three points in general position in three dimensions. For example both the following curves pass through the points $(1, 1, 0), (0, 0, 0), (1, 0, 1)$

$$\begin{cases} x - y - z = 0 \\ y^2 - y = 0 \\ z^2 - z = 0 \\ yz = 0 \end{cases} \quad \begin{cases} z + y - x = 0 \\ y^2 - y = 0 \\ yx - y = 0 \\ x^2 - x = 0. \end{cases} \quad (2.1)$$

Definition 13 *The affine variety of an ideal I is defined as*

$$\mathbf{V}(I) = \{(a_1, \dots, a_d) \in k^d : f(a_1, \dots, a_d) = 0 \text{ for all } f \in I\}.$$

For $I = \langle f_1, \dots, f_s \rangle$ we write $\mathbf{V}(I) = \mathbf{V}(f_1, \dots, f_s)$.

This definition is valid because of the Hilbert basis theorem. In general the ideal I generated by f_1, \dots, f_s is a subset of the ideal of the variety generated by f_1, \dots, f_s and this inclusion may be strict, for example $\langle x^2, y^2 \rangle \subsetneq I(\mathbf{V}(x^2, y^2)) = \langle x, y \rangle$. In symbols $I \subset I(\mathbf{V}(I))$. The relationship between $\langle f_1, \dots, f_s \rangle$ and $I(\mathbf{V})$ is fully explained by the Hilbert's Nullstellensatz (zero-place-theorem). In particular it gives the only reason why the inclusion might be strict for algebraically closed fields.

Theorem 5 (Hilbert's Nullstellensatz) *Let the coefficient field be algebraically closed. A polynomial f is in $I(\mathbf{V}(f_1, \dots, f_s))$ if there exists an integer $m \geq 1$ such that $f^m \in \langle f_1, \dots, f_s \rangle$.*

Theorem 6 (Strong Nullstellensatz) *Let the coefficient field be algebraically closed. For every ideal $I \in k[x_1, \dots, x_d]$, it holds that $I(\mathbf{V}(I)) = \sqrt{I}$, that is $I(\mathbf{V}(I))$ is radical.*

The Strong Nullstellensatz implies that two ideals generate the same variety if and only if their radicals are equal. A detailed explanation in one-dimension is useful. In one-dimension the Nullstellensatz becomes the algebraic closure for polynomials over algebraically closed fields, say over the complex numbers \mathbb{C} . Any polynomial ideal $I = \langle f_1, \dots, f_s \rangle \subset \mathbb{C}[x]$ is principal (that is generated by one element) and in particular $f = \text{GCD}(f_1, \dots, f_s)$ is a basis for I . Since \mathbb{C} is algebraically closed f is uniquely factorised as $f = c(x - a_1)^{r_1} \dots (x - a_p)^{r_p}$ for some $c, a_i \in \mathbb{C}$ and $r_i \in \mathbb{Z}_+$, $i = 1, \dots, p$. The square-free part of f is $f_{red} = c(x - a_1) \dots (x - a_p)$. Then $\mathbf{V}(f_1, \dots, f_s) = \mathbf{V}(f) = \{a_1, \dots, a_p\}$ and the Strong Nullstellensatz becomes $I(\mathbf{V}(f_1, \dots, f_s)) = I(\mathbf{V}(f)) = \langle f_{red} \rangle$. Without explanations that will draw us further afield we say that varieties containing only finitely many points are called zero-dimensional varieties. For the exact definition of dimension of a variety we refer to the standard texts, for example see Cox, Little and O'Shea (1992) [24]. Here we

simply say that the dimension of a finite set of points is zero, the dimension of a curve is one and of a surface is two.

The connection between varieties and radical ideals is so strong that an algebra-geometry dictionary has been made. The parts of this dictionary we shall use, taken from Cox, Little and O'Shea (1992) [24], are shown in Table 2.2. We suppose that the ideals involved are radical and the coefficient field is algebraically closed.

A design over $\mathcal{X} \in k^d$ can be interpreted as a variety and the design ideal is well-defined as the ideal of the variety. That is the set of all polynomials through the design points. Pointwise designs are thus zero-dimensional varieties. In Chapter 3 we see how to build the design ideal for pointwise designs.

2.3 Gröbner bases and the Buchberger algorithm

The Hilbert basis theorem states that any ideal is finitely generated, even if the generating set is not necessarily unique. Constructive proofs of the Hilbert basis theorem and of the Dickson's Lemma can be given in the forms of algorithms. In particular they give a special type of bases, the so-called Gröbner bases. The concept of leading term is again essential.

Definition 14 Given a term ordering τ on $k[x]$, a subset $G = \{g_1, \dots, g_t\}$ of an ideal I is a Gröbner basis if and only if

$$\langle Lt_\tau(g_1), \dots, Lt_\tau(g_t) \rangle = \langle Lt_\tau(I) \rangle$$

where $Lt_\tau(I) = \{Lt_\tau(f) : f \in I\}$.

Unless $\{g_1, \dots, g_t\}$ is a Gröbner basis, the following inclusion

$$\langle Lt(g_1), \dots, Lt(g_t) \rangle \subset \langle Lt(I) \rangle$$

may be strict, as the following example shows. Let $\langle x^3 - 2xy, x^2y - 2y^2 + x \rangle$ be an ideal in $\mathbb{Q}[x, y]$ with the $\text{tdeg}(x > y)$ ordering. It holds that $x^2 \in \langle Lt(I) \rangle$ but $x^2 \notin \langle Lt(x^3 - 2xy), Lt(x^2y - 2y^2 + x) \rangle$.

The Hilbert basis theorem provides the following theorem.

Theorem 7 Every ideal except $\{0\}$ has a Gröbner basis and any Gröbner basis is a basis.

Patently in the one-dimensional case a Gröbner basis of $I = \langle f_1, \dots, f_s \rangle$ is $\text{GCD}(f_1, \dots, f_s)$ with respect to the only term ordering for one-dimensional monomials, that is $1 < x < x^2 < x^3 < \dots$

In the definition of a Gröbner basis we cannot relax the requirement for a fixed term ordering as the following Maple output confirms. The Maple command `gbasis` returns the Gröbner basis of the specified ideal with respect to the given ordering. The orderings available in Maple are `lex` (called `plex`) and the total degree reverse lexicographic ordering (called `tdeg`).

```
> F := [x^2 - 2*x*z + 5, x*y^2 + y*z^3, 3*y^2 - 8*z^3]:
```

```
> gbasis(F, [y, x, z], plex);
```

```
[3*y^2 - 8*z^3, 80*y*z^3 - 3*z^8 + 32*z^7 - 40*z^5, x^2 - 2*x*z + 5,
-96*z^7 + 9*z^8 + 120*z^5 + 640*z^3*x, 240*z^6 + 1600*z^3 - 96*z^8 + 9*z^9]
```

```
> gbasis(F, [y, x, z], tdeg);
      [x2 - 2xz + 5, -3y2 + 8z3, 8xy2 + 3y3]
```

An ideal can have different Gröbner bases with respect to the same ordering. Both $\{y^2 - yx, x^2\}$ and $\{x^2 - xy + y^2, y^2 - xy\}$ are Gröbner bases with respect to $\text{tdeg}(x > y)$ of the same ideal. We shall see that given a term ordering an ideal has a unique *reduced* Gröbner basis.

The link between Gröbner bases and the division algorithm is expressed by the following theorem.

Theorem 8 *Let $I \subset k[x]$ be an ideal, τ a term ordering, $G = \langle g_1, \dots, g_s \rangle$ a Gröbner basis for I and $f \in k[x]$. Then there exist a unique remainder $r \in k[x]$ and a polynomial $g \in I$ such that (i) $f = g + r$ and (ii) no term of r is divisible by one of $Lt(g_1), \dots, Lt(g_s)$.*

Proof. The existence of g and r follows from the algorithm division with respect to the Gröbner basis. The uniqueness is proved by contradiction. Let $f = r_1 + g_1 = r_2 + g_2$, then $r_1 - r_2 = g_2 - g_1 \in I$. In particular $Lt(r_1 - r_2) \in \langle Lt(I) \rangle = \langle Lt(g_1), \dots, Lt(g_s) \rangle$ since G is a Gröbner basis. That is $Lt(r_1 - r_2)$ is divisible by some of the $Lt(g_i)$ but this is impossible since no term of r_1 and no term of r_2 has this property. Thus $r_1 - r_2 = 0$ and $r_1 = r_2$. The uniqueness of g follows from that of r . ■

Unfortunately the uniqueness of the remainder r does not imply the uniqueness of the decomposition over a Gröbner basis as the following example shows. The set $\{y - z, x + z\}$ is a Gröbner basis in $k[x, y, z]$ with respect to any ordering (Gröbner bases with this property are called *universal* Gröbner bases). The following two identities prove the assertion

$$\begin{aligned} xy &= y(x + z) + (-z)(y - z) + (-z^2) \\ xy &= x(y - z) + (+z)(x + z) + (-z^2). \end{aligned}$$

A most important consequence of Theorem 8 is the ideal membership test.

Corollary 1 *Let I be an ideal in $k[x]$, G be a Gröbner basis of I and f a polynomial in $k[x]$. Then $f \in I$ if and only if $\text{Rem}(f, G) = 0$.*

Definition 15 *A minimal Gröbner basis is a Gröbner basis such that (i) $Lc(g) = 1$ for all $g \in G$ and (ii) for all $g \in G$, $Lt(g)$ does not lie in $\langle Lt(G - \{g\}) \rangle$.*

A minimal Gröbner basis is a minimal basis in the sense that none of its proper subsets is a basis for the ideal.

Definition 16 *A reduced Gröbner basis is a Gröbner basis such that (i) $Lc(g) = 1$ for all $g \in G$ and (ii) for all $g \in G$, no term of g lies in $\langle Lt(G - \{g\}) \rangle$.*

Basically any term of any polynomial in a reduced Gröbner basis is essential. Clearly a reduced Gröbner basis is minimal.

Theorem 9 *Given a term ordering, any non-empty ideal I of $k[x]$ has a unique reduced Gröbner basis.*

Proof. Uniqueness: let G_1 and G_2 be two reduced Gröbner bases of I . By definition (in particular point (ii) in Definition 16) they have the same number of elements and the sets of their leading terms coincide: $Lt(G_1) = Lt(G_2)$. In particular for all $g_1 \in G_1$ there exists $g_2 \in G_2$ such that $Lt(g_1) = Lt(g_2)$ and this is a one-to-one correspondence. We have to prove $g_1 = g_2$. On the one hand since $g_1 - g_2 \in I$ we have $Rem(g_1 - g_2, G_1) = 0$. On the other hand none of the terms in $g_1 - g_2$ is divisible by any of the leading terms of the G_1 . This implies $Rem(g_1 - g_2, G_1) = g_1 - g_2$ and concludes the proof of the uniqueness of reduced Gröbner bases.

Existence: shortly we shall give algorithms computing minimal and reduced Gröbner bases. ■

For the proof of the following theorem we refer to Adams and Loustaunau, 1994 [1].

Theorem 10 *Let I be an ideal in $k[x]$, τ a term ordering and $G = \{g_1, \dots, g_t\} \subset I$. The following statements are equivalent.*

1. $G = \{g_1, \dots, g_t\}$ is a Gröbner basis for I .
2. For all $f \in I \setminus \{0\}$ there exists an element $g_i \in G$ such that $Lt(g_i)$ divides $Lt(f)$.
3. $\langle Lt(I) \rangle = \langle Lt(G) \rangle$.
4. For all $f \in I$ we have $Rem(f, G) = 0$ (ideal membership).
5. Any element $f \in I$ is decomposed over G in the following way

$$f = \sum_{i=1}^t f_i g_i \quad \text{and} \quad Lt(f) = \max(Lt(f_i) Lt(g_i)).$$

6. For any polynomial $f \in k[x]$ there exists unique $Rem(f, G)$ (remainder theorem).

2.3.1 The Buchberger algorithm

The ideal description problem is solved once we have an algorithm to compute Gröbner bases. This is the Buchberger algorithm. A major tool for the Buchberger algorithm is the so-called S -polynomial. In particular S -polynomials are used to test whether a set of polynomials is a Gröbner basis.

Definition 17 *Let f and g be polynomials in $k[x_1, \dots, x_d]$, τ a term ordering and $x_1^{\gamma_1} \dots x_d^{\gamma_d}$ the least common multiple (LCM) of $Lt(f)$ and $Lt(g)$. Then the S -polynomial of f and g is defined as*

$$S(f, g) = \frac{x_1^{\gamma_1} \dots x_d^{\gamma_d}}{Lm(f)} f - \frac{x_1^{\gamma_1} \dots x_d^{\gamma_d}}{Lm(g)} g.$$

Simply, $S(f, g)$ is the mechanism by which we cancel leading terms to produce the decomposition of Item 5 in Theorem 10. It is proved (Cox, Little and O'Shea, 1992 [24], Ch. 2 Lemma 5) that every cancellation of leading terms among polynomials of the same multi-degree involves S -polynomials. When considering two

polynomials at a time, this can be interpreted as a different way to compute the S -polynomial itself. For example $z(2x^3 + z) - 2x(x^2z + y^2) = z^2 - 2xy^2$ is equal to $2S(2x^3 + z, x^2z + yz) = \frac{x^3z}{2x^3}(2x^3 + z) - \frac{x^3z}{x^2z}(x^2z + y^2)$.

Let us detail how S -polynomials arise in the division algorithm. We want to divide f by f_1, \dots, f_s . In the division algorithm it may happen that both $Lt(f_i)$ and $Lt(f_j)$ divide the leading term X of f for some $i \neq j$. If we divide X by f_i then we have $h_1 = f - \frac{X}{Lt(f_i)}f_i$. If we divide X by f_j then we have $h_2 = f - \frac{X}{Lt(f_j)}f_j$ and an ambiguity introduced, that is the reason why the decomposition of Item 5 in Theorem 10 may not be unique, is

$$h_2 - h_1 = \frac{X}{Lt(f_i)}f_i - \frac{X}{Lt(f_j)}f_j = \frac{X}{LCM(Lt(f_j), Lt(f_i))}S(f_i, f_j).$$

Theorem 11 *A basis $G = \{g_1, \dots, g_s\}$ of an ideal I is a Gröbner basis if and only if for each pair (i, j) , $i, j \in \{1, \dots, s\}$*

$$Rem(S(g_i, g_j), G) = 0.$$

Theorem 11, for the proof of which we refer to for example Cox, Little and O'Shea (1992) [24], gives a finite test to verify whether a set of polynomials is a Gröbner basis.

Up to now we have seen that any ideal except $\{0\}$ has a Gröbner basis and that it has a unique reduced Gröbner basis. We present a three part version of the Buchberger algorithm which computes the reduced Gröbner basis of an ideal given a finite generating set and a term-ordering τ . The first part returns a Gröbner basis for the ideal, the second one makes it minimal and third one makes it reduced. Consistency, finiteness and correctness are proved in the literature (see for example Becker, Weispfenning and Kredel, 1991 [8]).

Input	$F = (f_1, \dots, f_s)$
Output	$G = (g_1, \dots, g_t) \supset F$ Gröbner basis
$G := F$	
REPEAT	
	$G1 := G$
	for each pair (p, q) $p \neq q$ in $G1$ do
	$S := Rem(S(p, q), G1)$
	if $S \neq 0$ then $G := G \cup \{S\}$
until $G = G1$	

Input	$G = (g_1, \dots, g_t)$ Gröbner basis
Output	$M = (m_1, \dots, m_u)$ minimal Gröbner basis
$M := G$	
for all $f \in M$ do	
	if $Lt(f) \in \langle Lt(M - \{f\}) \rangle$ then $M := M - \{f\}$
return M	

Input	$M = (m_1, \dots, m_u)$ minimal Gröbner basis
Output	$R = (r_1, \dots, r_v)$ reduced Gröbner basis
$R := M$	
for all $g \in R$ do	
	$g1 := \text{Rem}(g, R - \{g\})$
	$R := (R - \{g\}) \cup \{g1\}$
return R	

There are many ways to improve the above algorithm based both on sophisticated programming and additional mathematical ideas (for example the Gebauer-Möller formulae, see [12, 16, 46]).

Broadly speaking the Buchberger algorithm is a generalisation of the Gaussian elimination or row reduction algorithm for linear systems, as the following example in Maple shows

```
> A := matrix(3,4, [3,-6,-2,0,2,-4,0,4,1,-2,-1,-1]);
```

$$A := \begin{bmatrix} 3 & -6 & -2 & 0 \\ 2 & -4 & 0 & 4 \\ 1 & -2 & -1 & -1 \end{bmatrix}$$

```
> B:=gaussjord(A, 'r');
```

$$B := \begin{bmatrix} 1 & -2 & 0 & 2 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

```
> Id:=evalm( A &* [x,y,z,w] ): F:=[Id[1],Id[2],Id[3]];
> Id:=evalm( B &* [x,y,z,w] ): G:=[Id[1],Id[2]];
F := [3x - 6y - 2z, 2x - 4y + 4w, x - 2y - z - w]
G := [x - 2y + 2w, 3w + z]
```

```
F := [3x - 6y - 2z, 2x - 4y + 4w, x - 2y - z - w]
```

$$G := [x - 2y + 2w, 3w + z]$$

```
> gbasis(F, [x,y,z,w], plex);
```

$$[x - 2y + 2w, 3w + z]$$

The point is that F and G generate the same ideal, since the rows of B are obtained by those of A with ideal operations, and using the S -polynomial test we see that a reduced echelon matrix can only lead to a reduced Gröbner basis. For a discussion on the links between Gröbner bases and systems of linear equations we refer to Becker and Weispfenning, 1991 [8], §10.5 and Mora, 1994 [47].

2.4 Elimination theory

An immediate consequence of the above analysis is the use of Gröbner bases with the *lex* ordering to solve systems of linear equations. The use of Gröbner bases to solve systems of equations is called elimination theory (see also Section 2.1.4). It can be considered as a generalization to polynomial system of the Gaussian elimi-

nation for linear systems. A main theorem used in elimination theory is the Weak Nullstellensatz.

Theorem 12 (Weak Nullstellensatz) *Let k , the coefficient field, be algebraically closed then $V(I) = \emptyset$ if and only if $I = k[x_1, \dots, x_d]$.*

The problem of whether a system of polynomial equations $f_1 = \dots = f_s = 0$ has a solution is called the *consistency* problem. In terms of varieties this is equivalent to ask whether the varieties $V(f_1, \dots, f_s)$ is empty or not. Because of the Weak Nullstellensatz Theorem and the uniqueness of reduced Gröbner bases, over algebraically closed fields there is no solution to the system if and only if the reduced Gröbner basis of the system is $\{1\}$. In a non-algebraically closed field the condition is sufficient but non necessary, a counter example is that $1 + x^2 = 0$ has no solution in \mathbb{R} but $\{x^2 + 1\}$ is a reduced Gröbner basis.

Basically the elimination theory says that to solve the polynomial system of equation $f_1 = \dots = f_s = 0$ one can first find a reduced Gröbner basis of the ideal $\langle f_1, \dots, f_s \rangle$ with respect to the *lex* ordering. Call this $\{g_1, \dots, g_t\}$. The new system of equations $g_1 = \dots = g_t = 0$ has essentially a triangular form, which can be solved by backward substitution, and the two systems have the same solutions. In general the computation of the Gröbner basis with respect to the ordering *lex* is very expensive and there are methods to speed the computation based on the Hilbert function for polynomials (see Cox, Little and O'Shea, 1992 Chapter 9 [24]) implemented in the packages we use. For a reference see Traverso (1996) [71].

Examples of applications of elimination theory will be given in Chapter 3 where it is an essential tool in the construction of design ideals.

2.5 Polynomial functions and quotients by ideals

Quotients by ideals play a key role in the algebraic theory of identifiability of Chapter 3. The ring-isomorphism between polynomial functions over a variety and quotients by the variety ideal justifies the theory.

Definition 18 *Let $V \subset k^d$ be a variety. A function*

$$\Phi : V \longrightarrow k$$

is a polynomial function (or mapping) if there exists a polynomial $f \in k[x_1, \dots, x_d]$ such that

$$\Phi(a_1, \dots, a_d) = f(a_1, \dots, a_d)$$

for all (a_1, \dots, a_d) in V . The polynomial f is said to represent Φ . The collection of polynomial functions over V is denoted by $k[V]$.

Notice that two polynomial f and $g \in k[x]$ represent the same polynomial function on V if and only if $f - g \in I(V)$.

The set $k[V]$ is an Abelian ring with the following operations:

$$\begin{aligned} (\Phi + \Psi)(a) &= \Phi(a) + \Psi(a) \\ (\Phi \cdot \Psi)(a) &= \Phi(a) \cdot \Psi(a) \\ (\alpha\Phi)(a) &= \alpha(\Phi(a)). \end{aligned}$$

Moreover if f represents Φ and g represents Ψ then $f + g$ represents $\Phi + \Psi$ and $f \cdot g$ represents $\Phi \cdot \Psi$.

Definition 19 Let I be an ideal in $k[x]$. The quotient of $k[x]$ modulo I is defined as

$$k[x]/I = \{[f] : f \in k[x]\}$$

where $[f] := \{g \in k[x] \text{ such that } f - g \in I\}$.

The set $k[x]/I$ has the algebraic structure of a k -algebra. For all f and g in I and a scalar α in k we have

$$\begin{aligned} [f] + [g] &:= [f + g] \\ [f][g] &:= [fg] \\ \alpha[f] &:= [\alpha f]. \end{aligned}$$

If the ideal I is generated by a variety V , then we have that $f \equiv g$ modulo $I(V)$ if and only if f and g define the same polynomial function V . This connection is exploited in the next theorem.

Theorem 13 The sets $k[x]/I(V)$ and $k[V]$ are k -algebra isomorphic.

For the proof see Cox, Little and O'Shea Theorem 7 Chapter 5.

The division algorithm allows us to produce simple representations of equivalence classes for congruence modulo an ideal and thus for the set of polynomial functions over a variety. The next theorem reinterprets the division and the form of the remainder in this context. For the proof see Cox, Little, O'Shea Proposition 1 Chapter 5.

Theorem 14 Let a term ordering be fixed on $k[x]$ and let I be an ideal in $k[x]$.

1. Every $f \in k[x]$ is congruent modulo I to a unique polynomial r which is a k -linear combination of the monomials in the complement of the monomial ideal $\langle Lt(I) \rangle$.
2. The elements of $BG = \{x^\alpha : x^\alpha \notin \langle Lt(I) \rangle\}$ are linearly independent modulo I , that is modulo I

$$\sum_{x^\alpha \in BG} c_\alpha x^\alpha \equiv 0 \quad \text{with } c_\alpha \in k$$

if and only if $c_\alpha = 0$ for all α .

That is $k[x]/I$ is isomorphic as k -vector space to

$$BG = \text{Span}(x^\alpha : x^\alpha \notin \langle Lt(I) \rangle).$$

Different term orderings give different bases for BG . But they have all the same cardinality since $\text{Span}(x^\alpha : x^\alpha \notin \langle Lt_\tau(I) \rangle)$ are all k -vector spaces isomorphic to $k[x]/I$. For example the left system of polynomial equations in (2.1) gives a Gröbner basis with respect to the $\text{lex}(z < y < x)$ term ordering and the right one is a Gröbner basis with respect to the $\text{lex}(x < y < z)$ term ordering. Of course they represent the same ideal I . In both cases the dimension as a \mathbb{Q} -vector space of $\mathbb{Q}[x, y, z]/I$ is 3. On the left hand side BG is $\{1, z, y\}$ and on the right hand side it is $\{1, x, y\}$. Finally we state Theorem 15.

Geometry	Algebra
V	$I(V)$
$V \cap W$	$\sqrt{I(V) + I(W)}$
$V \cup W$	$\sqrt{I(V) \cdot I(W)}$
$V \cup W$	$I(V) \cap I(W)$
$\pi_h(V(I))^\dagger$	$\sqrt{I \cap k[x_{h+1}, \dots, x_d]}$

$\dagger \pi_h$ is the projector over the last $d - k - 1$ variables

Table 2.2: The algebra-geometry dictionary.

Theorem 15 Fix a term ordering on $k[x_1, \dots, x_d]$ and let k be algebraically closed. Let $V = V(I)$ be a variety over $k[x_1, \dots, x_d]$ and G a Gröbner basis for I . The following statements are equivalent. (i) V is finite. (ii) For each $i = 1, \dots, d$ there is $m_i \geq 0$ and $g \in G$ such that $x_i^{m_i} = Lm(g)$. (iii) The k -vector space $k[x_1, \dots, x_d]/I$ is finite-dimensional.

Theorem 15 characterises zero-dimensional ideals. In particular it follows that algorithmically the operation over $k[x]/I$ can be performed via Gröbner bases and the remainder theorem (Theorem 10 Item 6). For example let G be a Gröbner basis for I then $[f + g] = Rem(f + g, G)$ modulo I .

Summary

In this chapter we present the theory of Gröbner bases and its major links to algebraic geometry. The focus is on the concepts most relevant for the statistical application of the next chapters. The relevance of algebraic geometry to experimental design in the first instance stems from the fact that classical experimental designs are for polynomial models so that the ring of polynomials is central. In particular we consider the division algorithm, the duality between polynomial ideals and varieties and the Buchberger algorithm. The need for an algorithm such as the Buchberger algorithm is due to the non-uniqueness of division for polynomials in more than one variable.

Chapter 3

Design varieties and identifiability

In this chapter we present methods of algebraic geometry applied to the identifiability problem in experimental design: given a design which model(s) can we identify? Much of the foundation of our approach has been given in Chapter 2. The main purpose of the thesis is to develop this from the statistical point of view. The starting point is to represent the design as a variety, namely the solution of a set of algebraic equations. An equivalent description is the design ideal that is the set of all polynomials interpolating the design points. Starting with a class of models M (usually M will be the set of all polynomials in d indeterminates) the quotient vector space $M/I(V)$ yields a class of identifiable terms. The theory of Gröbner bases is used to characterise the design ideal and the quotient space.

The following problems will be addressed in particular (i) Which classes of polynomial models does a given design identify (direct problem)? (ii) Is a given model identifiable by a given design? (iii) What is confounding/aliasing in this context? (iv) How do we estimate the parameters? (v) What conditions must M satisfy so that the theory applies?

This algebraic approach to identifiability in experimental design was introduced by Pistone and Wynn in *Generalised Confounding with Gröbner Bases* (Biometrika 83,3:653–666, 1996). See the introductory chapter for details.

Other problems have been studied during this work by other authors. In particular Fontana, Pistone, Rogantin (1997, [31]) studied two-level designs and Caboara and Robbiano (1997, [15]) studied the inverse problem, that is: which fractions of the full factorial design estimate a given model.

3.1 The design variety

Definition 20 *A design is a zero-dimensional variety, V .*

From a statistical point of view a design is a pointwise finite subset without replication in a d -dimensional design space $\mathcal{X} \subset k^d$, equivalently a single replicate design. We are interested in the design ideal $I(V)$.

The starting point is to replace a design by its equivalent variety and then by the ideal associated to the variety. In the language of algebraic geometry a zero-

dimensional variety is generated by the radical ideal containing a polynomial interpolating the points. As an example, the 2^2 full factorial design $\{(\pm 1, \pm 1)\}$ corresponds to the ideal

$$\langle (x-1)(x+1), (y-1)(y+1) \rangle = \langle x^2 - 1, y^2 - 1 \rangle \subset \mathbb{Q}[x, y].$$

A Gröbner basis is an alternative representation of the design ideal which has useful properties (see Theorem 14) and assumes a term ordering. Thus we have different Gröbner basis representations of the same ideal corresponding to different term orderings. Let us give an interpretation in terms of interpolation. For clarity we use the two dimensional space. Given a set of points in the plane (x, y) with distinct x values we can always find the unique polynomial of minimum degree $y = p(x)$ through these points. In higher dimension this is no longer true. Unless we fix an ordering which, roughly speaking, determines which point to fit first. Gröbner basis theory deals exactly with this problem. Given the design points x_i and the observed values $Y_i = p(x_i)$, for $i = 1, \dots, N$, the remainder of p with respect to the Gröbner basis through the $(x_i, Y_i)_{i=1, \dots, N}$ is the minimum polynomial (with respect to the ordering) through those points.

There are various ways to construct the design ideal. An efficient method is based on specialised linear algebra techniques for zero-dimensional ideals (see Marinari, Möller, Mora, 1996 [46]). It has recently been implemented in CoCoA by Dr. A. Bigatti at Genova University and in Reduce by Mr. R. Tenberg at Dortmund University (personal communications). Next we present two less sophisticated but more intuitive methods to determine the design ideal given the affine coordinates of the design points.

The first method is a direct application of elimination theory and we introduce it with an example. The 2^2 -full factorial variety is given by the projection in $\mathbb{Q}[x, y]$ of the following 6-dimensional ideal

$$\langle t_1(x-1), t_1(y-1), t_2(x+1), t_2(y-1), \\ t_3(x-1), t_3(y+1), t_4(x+1), t_4(y+1), t_1 + t_2 + t_3 + t_4 - 1 \rangle.$$

The last polynomial excludes unwanted points given by $t_i = 0$ ($i = 1, \dots, 4$). The following Maple output shows the procedure.

```
> design := [t1*(x-1), t1*(y-1), t2*(x+1), t2*(y+1), t3*(x+1), t3*(y-1),
> t4*(x-1), t4*(y+1), t1+t2+t3+t4-1]:
> Variables := [t1, t2, t3, t4, x, y]:
> BigBasis := gbasis(design, Variables, plex);
BigBasis := [4 t1 - y x - x - 1 - y, 4 t2 + y x - x + y - 1,
4 t3 + x - 1 + y x - y, 4 t4 - y x + y + x - 1, x^2 - 1, y^2 - 1]

> DesignIdeal := [ BigBasis[ nops(BigBasis)-1 .. nops(BigBasis) ] ];
DesignIdeal := [ x^2 - 1, y^2 - 1 ]
```

In d -dimensions the N -point variety

$$(a_{1_1}, \dots, a_{1_d}), \dots, (a_{N_1}, \dots, a_{N_d})$$

is the set of the (real) zeros of the N -elimination ideal of the following ideal in $N + d$ variables

$$I = \langle t_i(x_j - a_{ij}) : i = 1, \dots, N, j = 1, \dots, d, \\ t_1 + \dots + t_N - 1 \rangle \subset \mathbb{Q}[t_1, \dots, t_N, x_1, \dots, x_d].$$

We recall that the N -elimination ideal of $I \subset \mathbb{Q}[\theta, \mathbf{x}]$ is $I \cap \mathbb{Q}[\mathbf{x}]$. The procedure is summarised in the following algorithm.

1. Write $I \subset \mathbb{R}[t_1, \dots, t_N, x_1, \dots, x_d]$.
2. Find a Gröbner basis G for I with respect to lex in $\mathbb{R}[t_1, \dots, t_N, x_1, \dots, x_d]$.
3. The elements of G not involving the t_i 's variables are the reduced Gröbner basis for $I \cap \mathbb{R}[x_1, \dots, x_d]$ with respect to lex .

This method can be implemented in any computer algebra package which computes Gröbner bases with respect to the lexicographic term-ordering. In CoCoA this procedure is given by the built-in function `Elim`. Once we have a Gröbner basis of an ideal with respect to a term ordering the Gröbner basis with respect to another term ordering can be computed with the Buchberger algorithm.

Another method to compute design ideal is based on the fact that finite unions of varieties correspond to finite intersections of ideals in the algebra-geometry dictionary. That is $V_1 \cup V_2$ corresponds to $I(V_1) \cap I(V_2)$. We write this as $I(V_1 \cup V_2) = I(V_1) \cap I(V_2)$. In particular a pointwise design is the finite union of its design points. The point with coordinates (a_1, \dots, a_d) corresponds to the ideal $I((x_1 - a_1), \dots, (x_d - a_d))$. The intersection of all the single point ideals gives the ideal corresponding to the whole design. Some computer algebra packages, including CoCoA, provide an efficient built-in procedure to calculate Gröbner bases of intersection of ideals. The algorithm is as follows.

1. Consider the reduced Gröbner basis of the single point design ideal $(x_1 - a_1, \dots, x_n - a_n)$.
2. Intersect the single point design ideals over all the design points.

We implemented the above algorithm in the CoCoA function called `DesignIdeal` (see Table 3.1) which takes as input the coordinates of the design points and returns the reduced Gröbner basis of the design ideal with respect to the term ordering specified at the start of the CoCoA session. As an example consider again the 2^2 -full factorial.

```
Use T:=Q[xy], DegRevLex;
Design:=[ [0,0], [0,1], [1,0], [1,1] ];
DesignIdeal(Design);
Ideal(y^2 - y, x^2 - x)
```

3.1.1 Examples

In this section we compute the reduced Gröbner bases for various design ideals. We start with the full-factorial design. The 3^3 -full factorial with three factors at levels


```

// Input: a list of numbers with as many element as indeterminates.
// Output: the reduced GB of the single point design ideal.
// N.B.: the term ordering is specified at the start of the session.
Define OnePointIdeal(P)
  If Len(P) <> NumIndets Then
    Return Error('Wrong number of indeterminates') End;
  F:=1; While F ≤ NumIndets And P[F]=0 Do
    F:=F+1; End;
  L:= [ Indet(K) - P[K] — K In 1..NumIndets];
  Return Ideal(L);
End;

// Input: a list of list (list of points = design).
// Output: the reduced GB of the ideal generated by that design.
// N.B.: the term ordering is specified at the start of the session.
Define DesignIdeal(L)
  I:=OnePointIdeal(Head(L));
  Foreach P In Tail(L) Do
    Catch J:=OnePointIdeal(P) In E End;
  If Type(E) = ERROR Then Print P, ':'; Return E End;
  I:=Intersection(I,J) End;
  Return I
End;

```

Table 3.1: CoCoA macros for design ideals.

$\{-1, 0, 1\}$ corresponds to the variety

$$V(x_1^3 - x_1, x_2^3 - x_2, x_3^3 - x_3).$$

In general the l^n -full factorial is represented by the variety

$$V(P_1(x_1), \dots, P_n(x_n))$$

where the P_i 's are square-free polynomials of degree l in the x_i 's and whose roots are the levels of the i -th factor. Notice that the symmetry of the design is transferred into the symmetry of the polynomial system defining/interpolating the design points. The identifiability problem is clearly invariant to scaling and shifting of the factors. For example shifting the levels from $\{-1, 0, 1\}$ to $\{0, 1, 2\}$ in the first variable x_1 corresponds to a shifting of x_1 giving in the above example $x_1^3 + 3x_1^2 + 2x_1$ instead of $x_1^3 - x_1$.

The fractional design obtained by the 3^3 -full factorial with at least one component zero is the intersection of the varieties $V(x^3 - z, y^3 - y, x^3 - x)$ and $V(xyz)$. Intersection of ideal varieties corresponds to sum of ideals, that is $V(I_1) \cap V(I_2)$ is $V(I_1 + I_2)$. These operations are implemented in CoCoA and the result is $(z^3 - z, y^3 - y, x^3 - x, xyz)$ with respect to any term ordering.

The term ordering becomes essential in the description of the ideal corresponding to the 3^{4-2} -fractional factorial with level $\{-1, 0, 1\}$. With respect to the `lex` ordering we have

$$\begin{aligned} &\text{Ideal}(t^3 - t, \\ &x + 9/4z^2t^2 - 3/4z^2t - 3/2z^2 + 3/4zt^2 + 3/4zt - 1/2z - 3/2t^2 + 1/2t + 1, \\ &z^3 - z, \\ &y - 3/2z^2t - 3/2zt^2 + z + t) \end{aligned}$$

and with respect to `tdeg` we have

$$\begin{aligned} &\text{Ideal}(xt - 1/2yt + 1/2zt + 1/2y + 1/2z, \\ &yz + z^2 - yt - t^2, \\ &xz - 1/2z^2 + 1/2yt - 1/2zt + 1/2t^2 + 1/2y + 1/2t, \\ &y^2 - z^2 + yt - zt, \\ &xy + 1/2z^2 - 1/2t^2 + 1/2z + 1/2t, x^2 + 2z^2 - 2yt - x - 2, \\ &z^2t + z^2 - yt - 2/3x - 1/3y - 2/3t - 2/3, \\ &z^3 - z, t^3 - t, \\ &zt^2 - z^2 + yt + 2/3x - 1/3y - 2/3z + 2/3, \\ &yt^2 + z^2 - yt - 2/3x - 2/3y - 1/3z - 2/3) . \end{aligned}$$

Caboara, Pistone, Riccomagno and Wynn (1997) [52] describe the so-called echelon designs. A design $D \subset Z_+^d$ is called an echelon design if for any design point (a_1, \dots, a_d) all points of the form (y_1, \dots, y_d) with $0 \leq y_j \leq a_j$, for all $j = 1, \dots, d$ belong to the design D . As an example consider in two dimensions the design

$$D = \{(0, 0), (1, 0), (2, 0), (3, 0), (0, 1), (1, 1), (2, 1), (0, 2)\}$$

with point pattern

$$\begin{aligned} &\cdot \\ &\cdot \cdot \cdot \\ &\cdot \cdot \cdot \cdot \end{aligned}$$

A (non reduced) Gröbner basis for the design ideal with respect to any term ordering is given by the following five polynomials

$$\begin{cases} x_2(x_2 - 1)(x_2 - 2) \\ x_1x_2(x_2 - 1) \\ x_1(x_1 - 1)x_2(x_2 - 1) \\ x_1(x_1 - 1)(x_1 - 2)x_2 \\ x_1(x_1 - 1)(x_1 - 2)(x_1 - 3). \end{cases}$$

Let now D be a generic echelon design in two dimensions. It is the union of columns of points of the form

$$\begin{aligned} (0, h) &: h = 0, \dots, k_0 \\ (1, h) &: h = 0, \dots, k_1 \\ &\vdots \\ (l, h) &: h = 0, \dots, k_l \end{aligned}$$

where $k_0 \geq k_1 \geq \dots \geq k_l$. Caboara, Pistone, Riccomagno and Wynn (1997) [52] prove that the following polynomials form a Gröbner basis for the design ideal

$$\begin{cases} p_0(x_2) = \prod_{j=0}^{k_0} (x_2 - j) \\ p_1(x_1, x_2) = x_1 \prod_{j=0}^{k_1} (x_2 - j) \\ p_2(x_1, x_2) = x_1(x_1 - 1) \prod_{j=0}^{k_2} (x_2 - j) \\ \vdots \\ p_l(x_1, x_2) = \prod_{j=0}^{l-1} (x_1 - j) \prod_{j=0}^{k_l} (x_2 - j) \\ p_{l+1}(x_1) = \prod_{j=0}^l (x_1 - j), \end{cases} \quad (3.1)$$

and extend it to higher dimensions. See also Robbiano and Rogantin (1997) [61].

3.2 Algebraic identifiability

In this section given a single replicate design D in d -dimensions and a term ordering τ over the terms of $k[x]$ we are interested in a saturated set of terms that defines an identifiable model. Theorem 14 of Chapter 2 is at the heart of the theory. It states that a saturated set of monomials identifiable by D with respect to the ordering τ is

$$Est_{D,\tau} = \{\mathbf{x}^\alpha : \mathbf{x}^\alpha \text{ is not divisible by any of the } Lt(\mathbf{I}(D))\}$$

where the term ordering defines $Lt(\mathbf{I}(D))$. If G is a Gröbner basis of D with respect to τ the set of identifiable terms can be determined as follows

$$Est_{D,\tau} = \{\mathbf{x}^\alpha : \mathbf{x}^\alpha \text{ is not divisible by any of the } Lt(g) \text{ such that } g \in G\}.$$

Thus the saturated model

$$\sum_{\mathbf{x}^\alpha \in Est_{D,\tau}} \theta_\alpha \mathbf{x}^\alpha$$

is unambiguously identifiable since at the design points \mathbf{x}_i and at the observed values Y_i , for all $\mathbf{x}_i \in D$, the linear system of equations

$$Y_i = \sum_{\mathbf{x}^\alpha \in Est_{D,\tau}} \theta_\alpha \mathbf{x}^\alpha(\mathbf{x}_i)$$

has one and only one solutions with respect to θ_α since the elements of $Est_{D,\tau}$ are the basis for a k -vector space where k is space of the coefficients, that is the space where the design point coordinates assume value. Any element of $Est_{D,\tau}$ is the representative of an equivalence class (congruent to the design ideal) and thus it can be substituted by any other element of the class, not necessarily a monomial.

An important consequence is that with a N point-design we can identify at most N distinct terms. Indeed by Theorem 14 we have that we can always identify the same number of terms whatever term ordering we use and by the elimination theory it follows that it must be N . While the dimension is independent of the orderings the elements of $Est_{D,\tau}$ strongly depend on the chosen ordering and thus we have a whole range of identifiable saturated sets (see also Section 3.3). This fact could be used to influence the model structure. For example when main effects are favoured then an ordering that respects the total degree of terms, such as the $tdeg$ ordering, may be used or when one effects dominates all the others then a lexicographic ordering may be most appropriate.

Note that $Est_{d,\tau}$ is an *order ideal* where E is an order ideal if (i) E is a finite set of monomials and (ii) if $x^\alpha \in E$ and x^β divides x^α then $x^\beta \in E$. In particular (ii) expresses a divisibility condition (D) that is if a term $x^\alpha = x_1^{\alpha_1} \dots x_m^{\alpha_m}$ is in $Est_{d,\tau}$ then every term which divides x^α is also in $Est_{d,\tau}$. For example if $x_1^2 x_2$ is in $Est_{d,\tau}$ then so are $x_1, x_2, x_1 x_2, x_1^2$ and the constant term, which is here given by 1. This reflects one common practice in modelling of including all the factors of a present interaction. Note that once we have determined the Gröber basis with respect to a given term ordering the set of identifiable terms is automatically defined since it only depends on the compatibility with monomial multiplication which any monomial ordering satisfies.

It is useful to consider the problem in terms of interpolation. Since the number of estimable terms is exactly the sample size we obtain *exact interpolation* when we fit the linear model composed exactly of identifiable terms. We can clearly fit any submodel we wish. It is important to emphasise that we start with the whole of $k[x]$. Recall that the vector space $k[x]/I(D)$ is the set of classes of remainders of the polynomials of $k[x]$ with respect to division by the Gröbner basis $G = \{f_1, \dots, f_v\}$ given a term ordering τ :

$$k[x]/I(D) := \{r \in k[x] : \text{there exist } f, q_1, \dots, q_v \in k[x] \text{ such that } f = \sum_{j=1}^v q_j f_j + r.\}$$

One interpretation is that the equivalence class of a certain polynomial f gives all the polynomials that interpolate the values of f at the design points.

With the above notation the concept of algebraic identifiability is summarised by the following mapping

$$\begin{aligned} \mathcal{I}_{D,\tau} : k(\theta_0, \dots, \theta_p)[x] &\longrightarrow k(\theta_0, \dots, \theta_p)[x]/I(D) \\ f &\longmapsto \text{Rem}(f, G) \end{aligned}$$

where we stress the presence of parameters in the coefficient field. Note that $\mathcal{I}_{D,\tau}$ is not the congruence modulo $I(D)$. Indeed it concentrates on the vector-space structure of the quotient ideal and the operation defining it is the division.

Given a model f , a term ordering τ and a design D a model identifiable by D and confounded to f is $\text{Rem}(f, G)$ where G is a Gröbner basis for $I(D)$ with respect

to τ . In particular if $Rem(f, G)$ is f then f is identifiable by D . Consider in three dimension the polynomial $x_3^2 - 1$. Its remainder with respect to $G = \{x_1^2 - 1, x_2^2 - 1\}$ is $x_3^2 - 1$ but f is not identifiable. This is because G is not the G-basis of a zero-dimensional ideal in three dimension. That is it does not generate a design ideal.

Thus the problem of checking whether a model is identifiable by a design consists of computing and checking a remainder. This operation can be carried out in CoCoA and Maple. The division algorithm operates linearly on the coefficients/parameters of f and thus on the parameters of the model in such a way that if f is identifiable with respect to a certain term ordering then it is identifiable with respect to any term ordering.

Each of the equivalence classes in $k[x]/I(D)$ can be interpreted as an aliasing class in the sense that only one term from each class can be part of the same identifiable model (see Pistone, Holliday, Riccomagno and Wynn, 1996 [37]). That is any residual class of $k[x]/I(D)$ is an infinite family of models which are not distinguishable by the design. Two models, f and g are confounded (aliased) under the design D if and only if $f - g$ belongs to the design ideal $I(D)$. This is the algebraic counterpart of aliasing: two polynomial models f and g are aliased under the design D if $\mathcal{I}_{D,\tau}(f) = \mathcal{I}_{D,\tau}(g)$. In particular the inverse image of $\mathcal{I}_{D,\tau}(f)$ gives the set of all polynomials aliased to f under the pair (D, τ) .

Given the design D this technique allows us to select identifiable models. Specifically select the regression vectors $X(\mathbf{x})$ as basis of the vector space $k[x]/I(D)$. The design matrix \mathbf{X} for such a model is invertible and given an observed vector \mathbf{Y} we have $\hat{\theta} = \mathbf{X}^{-1}\mathbf{Y}$ as usual. Thus algebraic estimability becomes the following mapping

$$\begin{aligned} \mathcal{I}_{D,\tau} : \mathbb{Q}(\theta_0, \dots, \theta_p)[x_1, \dots, x_d] \times \mathbb{Q}^N &\longrightarrow \mathbb{Q}[x_1, \dots, x_d]/I(D) \\ (f, \mathbf{Y}) &\longmapsto \mathbf{X}(\mathbf{x})(\mathbf{X}^t\mathbf{X})^{-1}\mathbf{X}^t\mathbf{Y} \end{aligned}$$

where $X(\mathbf{x})$ is the regression vector extracted from $Rem(f, G)$ and \mathbf{X} is the design matrix for $X(\mathbf{x})$ and D , and N is the design size. We consciously used the same notation for algebraic identifiability and estimability to stress that they often correspond both in theory and applications.

Our examples are based on the following algorithm which takes the design point coordinates as a list of lists and returns the full list of identifiable terms with respect to the specified term ordering.

1. Input a design D and a term ordering τ .
2. Compute the Gröbner basis.
3. Determine the identifiable terms as the order ideal $Est_{D,\tau}$.

3.2.1 Examples

In this section we find the set of identifiable terms for some design-term ordering pairs. We have worked out these examples in CoCoA and Maple. The set of terms estimable by the 3^3 -full factorial with respect to the tdeg term ordering is the following

$$Est = [x^2y^2z^2, x^2y^2z, x^2yz^2, xy^2z^2, x^2y^2, x^2yz, xy^2z,$$

```

// Input: a list of list (list of points = design),
//         the number of design points,
//         an integer M.
// Output: The set of estimable terms or the request of increasing M.
Define Identifiability(DesignCoord,P,M);
    DesignId:=DesignIdeal(DesignCoord);
    Lm:=[ LT(K) — K In DesignId ];
    Est:=OrderId(Lm,M);
    If Len(Est)=P Then Return Est
    Else Return Len(Est);
End;
End;

// Input: a list of monomials (leading terms).
// Output: the list of monomials not divisible by any element in the input list.
// N.B.: M is a positive integer. If M is too big then the function is slow.
//        If M is too small then not all the identifiable terms are captured.
Define OrderId(Lm,M);
    Model:=[1];
    For A:=1 To M Do
        Model:=Concat( Model, Monomials(DensePoly(A)) ) End;
    C:=NewList(Len(Lm),0);
    O:=[ X In Model — [Div(X,Y) — Y In Lm] = C ];
    Return O;
End;

```

Table 3.2: CoCoA macro for identifiability.

$$x^2z^2, xyz^2, y^2z^2, x^2y, xy^2, x^2z, xyz, y^2z, xz^2, \\ yz^2, x^2, xy, y^2, xz, yz, z^2, x, y, z, 1].$$

We have the well-known result that the largest model we can identify with the 3^3 -full factorial design is the standard quadratic model. This is actually true for all term ordering since the Gröbner basis $\{x^3 - x, y^3 - y, z^3 - z\}$ has the same leading terms with respect to any term ordering and the computation of *Est* does not depend on the term ordering. We call such a basis a *total* Gröbner basis.

The subset of 3^3 -full factorial with at least one zero-component gives the following subset of identifiable terms with respect to any term ordering.

$$Est = [x^2y^2, x^2z^2, y^2z^2, x^2y, xy^2, x^2z, y^2z, xz^2, yz^2, \\ x^2, xy, y^2, xz, yz, z^2, x, y, z, 1].$$

For the 3^{4-2} fractional full factorial design with tdeg ordering we have

$$Est_{3^{4-2}, \text{tdeg}} = [z^2, yt, zt, t^2, x, y, z, t, 1]$$

and with the lexicographic ordering for $x > y > z > t$

$$Est_{3^{4-2}, \text{lex}} = [z^2t^2, z^2t, z^2, zt^2, zt, z, t^2, t, 1].$$

As expected by the property of lexicographic ordering two factors x and y are not in the list of identifiable terms. Note here the fact that the cardinality of these last two sets is equal to 9, the number of design points.

We now consider the quadratic model in one-variable and the three point design $\{\alpha, \beta, \gamma\}$

```
> Design:=(x-alpha)*(x-beta)*(x-gamma);
      Design := (x - alpha)(x - beta)(x - gamma)

> Model:=a*x^2+b*x+c;
      Model := a x^2 + b x + c

> normalf(Model,[ Design ],[x],plex);
      a x^2 + b x + c
```

Being in one-dimension all the term orderings are equivalent. Thus we chose one arbitrarily in order to run the functions *gbasis* and *normalf* in Maple. As expected we find that all the 3-model parameters are identifiable. We would have had the same result even with replications for example $\alpha = \beta$ since the design is represented by a polynomial of third degree and the model by a second order polynomial. But the result would not have been reasonable. To check this we could try to estimate the parameters, that is solve the following system of equations

```
> syst:=a*alpha^2+b*alpha+c=Y1,a*alpha^2+b*alpha+c=Y2,
> a*gamma^2+b*gamma+c=Y3;
> A:=solve({syst},{a,b,c});
```

$A :=$

Maple cannot solve this system since it is an impossible system if $Y_1 \neq Y_2$ or it has

infinite¹ solutions if $Y_1 = Y_2$.

For the cubic model and the previous design we obtain that the linear and cubic effects are aliased

```
> Cubic:=a*x^3+b*x^2+c*x+d;
      Cubic := a x3 + b x2 + c x + d

> normalf(Cubic,Design,[x],plex);
      d + α β γ a + (c - a β γ - a α γ - a α β) x + (b + a γ + a β + a α) x2
```

An early example of the theory (see Pistone and Wynn, 1996 [53]) has a nice interpretation in terms of interpolation. Consider three points in generic position in the plane. In Maple we work out the Gröbner basis for the design ideal with respect to the lex ordering.

```
> # 3 points in general position in the plane
> design:=[ t1*(x-a1),t1*(y-b1), t2*(x-a2),t2*(y-b2),
> t3*(x-a3),t3*(y-b3),t1+t2+t3-1];
> GBasis:= gbasis( design,[t1,t2,t3,x,y],plex );
> Id:=[ seq( GBasis[i], i=4..5 ) ];

      Id := [-b3 a1 b22 + b32 a1 b2 + b3 a2 b12 - b32 a2 b1 + a3 b22 b1
      - a3 b2 b12
      + (a1 b22 - a1 b32 + a2 b32 - a2 b12 + a3 b12 - a3 b22) y
      + (-a1 b2 + a1 b3 - a2 b3 + a3 b2 + a2 b1 - a3 b1) y2
      + (b22 b3 - b2 b32 - b3 b12 + b32 b1 - b22 b1 + b2 b12) x,
      -b3 b2 b1 + (b2 b1 + b3 b1 + b2 b3) y + (-b1 - b2 - b3) y2 + y3]
```

Then we write the leading monomials and put in evidence their coefficients

```
> LMplex:=[seq( leadmon( Id[i],[x,y],plex)[2],
> i=1..nops(Id) ) ];
      LMplex := [ x, y3 ]

> LMcoeffplex:=[ seq( leadmon( Id[i],[x,y],plex)[1],
> i=1..nops(Id) ) ];
      LMcoeffplex := [ b22 b3 - b2 b32 - b3 b12 + b32 b1 - b22 b1 + b2 b12, 1 ]
```

The set of identifiable terms is

$$Est_{gen2,lex} := [1, y, y^2].$$

We notice that the coefficient of x is zero if and only if at least two of the design points have the same y value. Repeating the above procedure with respect to lex and with the constraint $b_1=b_2$ the set of leading terms becomes

$$LMplex := [xy, x^2]$$

Thus the identifiable terms are

$$Est_{gen2, b_1=b_2, lex} := [1, y, x].$$

The same result is obtained when the calculations are carried out with respect to tdeg ordering. This is an example of the connection between the structure of a

design and the set of identifiable terms. A major area of future work is to analyse the link between the geometry structure of designs and the set of identifiable terms returned by the above procedure for a fixed term ordering. Some initial results are contained in the study of fans in the next two sections.

We have seen that with the 3^3 -full factorial design we can estimate the standard quadratic model. Let us see the confounded structure for a standard cubic model under a 3^3 -full factorial.

```

> # Cubic standard model
> Lista:=[]:
> for i from 0 to 3 do for j from 0 to 3 do for k from 0 to 3 do
> Lista:=[op(Lista),[i,j,k] ];
> od; od; od;
> QuadModel:=p[0,0,0]:
> for P in Lista do
> QuadModel:=QuadModel+ p[P[1],P[2],P[3]] *x^P[1]*y^P[2]*z^P[3]
> od:
> assume(p,integer);
> # Design
> DesignIdeal:=[ x^3-x,y^3-y,z^3-z];

```

$$DesignIdeal := [x^3 - x, y^3 - y, z^3 - z]$$

```

> normalf(QuadModel,DesignIdeal,[x,y,z],tdeg);

```

$$\begin{aligned}
& (p_{2,1,0}^- + p_{2,3,0}^-) x^2 y + p_{2,0,2}^- x^2 z^2 + p_{2,0,0}^- x^2 + p_{2,2,0}^- x^2 y^2 \\
& + p_{2,2,2}^- x^2 y^2 z^2 + (p_{1,2,0}^- + p_{3,2,0}^-) x y^2 \\
& + (p_{2,0,1}^- + p_{2,0,3}^-) x^2 z + (p_{0,2,1}^- + p_{0,2,3}^-) y^2 z \\
& + (p_{1,0,2}^- + p_{3,0,2}^-) x z^2 \\
& + (p_{1,1,0}^- + p_{3,1,0}^- + p_{1,3,0}^- + p_{3,3,0}^-) x y \\
& + (p_{1,0,1}^- + p_{3,0,1}^- + p_{1,0,3}^- + p_{3,0,3}^-) x z \\
& + (p_{0,1,1}^- + p_{0,3,1}^- + p_{0,1,3}^- + p_{0,3,3}^-) y z \\
& + (p_{0,1,2}^- + p_{0,3,2}^-) y z^2 + (p_{0,1,0}^- + p_{0,3,0}^-) y \\
& + (p_{1,1,2}^- + p_{3,1,2}^- + p_{1,3,2}^- + p_{3,3,2}^-) x y z^2 + (p_{1,1,1}^- + p_{3,1,1}^- \\
& + p_{1,3,1}^- + p_{3,3,1}^- + p_{1,1,3}^- + p_{3,1,3}^- + p_{1,3,3}^- + p_{3,3,3}^-) x y z \\
& + (p_{2,1,2}^- + p_{2,3,2}^-) x^2 y z^2 + (p_{1,2,2}^- + p_{3,2,2}^-) x y^2 z^2 \\
& + (p_{2,1,1}^- + p_{2,3,1}^- + p_{2,1,3}^- + p_{2,3,3}^-) x^2 y z \\
& + (p_{1,2,1}^- + p_{3,2,1}^- + p_{1,2,3}^- + p_{3,2,3}^-) x y^2 z \\
& + (p_{2,2,1}^- + p_{2,2,3}^-) x^2 y^2 z + (p_{0,0,1}^- + p_{0,0,3}^-) z \\
& + (p_{1,0,0}^- + p_{3,0,0}^-) x + 2 p_{0,0,0}^- + p_{0,2,2}^- y^2 z^2 + p_{0,2,0}^- y^2 \\
& + p_{0,0,2}^- z^2
\end{aligned}$$

Of the 64 parameters of the cubic model only the 7 coefficient terms involving only second order powers and the constant are fully identifiable. Notice that the coefficients of the other identifiable terms are linear combinations of the model parameters. This is always the case since the division operates linearly on the coefficients of the dividend.

Another example is the standard quadratic model in 3 dimensions and the subset of 3^3 -full factorial with at least one zero-component.

```
> # Standard quadratic with subset of 3^3 with zeros
> with(grobner);
    [finduni, finite, gbasis, gsolve, leadmon, normalf, solvable, spoly]

> Lista:=[]:
> for i from 0 to 2 do for j from 0 to 2 do for k from 0 to 2 do
> Lista:=[op(Lista), [i,j,k] ];
> od; od; od;
> QuadModel:=p[0,0,0]:
> for P in Lista do
> QuadModel:=QuadModel+ p[P[1],P[2],P[3]] *x^P[1]*y^P[2]*z^P[3]
> od:
> assume(p,integer);
> # Design
> DesignIdeal:=[ x^3-x,y^3-y,z^3-z,x*y*z];
    DesignIdeal := [ x^3 - x, y^3 - y, z^3 - z, x y z ]

> Est:=normalf(QuadModel,DesignIdeal,[x,y,z],tdeg);
    Est := p~_{0,1,2} y z^2 + p~_{2,0,0} x^2 + p~_{0,2,0} y^2 + p~_{1,0,2} x z^2 + p~_{0,0,1} z
    + p~_{0,0,2} z^2 + p~_{1,1,0} x y + p~_{1,0,0} x + p~_{0,1,0} y + p~_{2,1,0} x^2 y
    + p~_{0,2,2} y^2 z^2 + p~_{0,1,1} y z + 2 p~_{0,0,0} + p~_{0,2,1} y^2 z + p~_{1,0,1} x z
    + p~_{1,2,0} x y^2 + p~_{2,0,1} x^2 z + p~_{2,0,2} x^2 z^2 + p~_{2,2,0} x^2 y^2

> nops(Est);
```

19

3.3 The fan of a design

In Section 3.2 given a design D and a term ordering τ we give a procedure to compute a saturated set of identifiable terms. In this section we look for all the saturated sets of identifiable terms as the term ordering τ spans over all the term orderings described in Definition 7 of Chapter 2. At first this looks like a search problem over the infinite set of monomial orderings, but in reality this is not the case. We refer to Caboara, Pistone, Riccomagno and Wynn (1997) [13] that introduces the notion of fan of a design following Robbiano and Mora (1988) [49].

Given a Gröbner basis, G of the ideal I with respect to a term ordering τ the monomial ideal generated by the leading terms of G is called the *initial ideal*

$$\text{Init}_\tau(G) = \langle \text{Lt}_\tau(g) : g \in G \rangle .$$

Notice that by the definition of a Gröbner basis the following holds

$$\text{Init}_\tau(G) = \langle \text{Lt}_\tau(g) : g \in I \rangle .$$

The set of all monomials not divisible by any of the $\text{Lt}(g)$, $g \in G$, that is the monomials not in $\text{Init}_\tau(G)$ is an order ideal.

The following is proved for example in Sturmfels (1995) [70]: *every ideal $I \subset k[x]$ has only finitely many distinct initial ideals, equivalently order ideals.* This allows us to define an equivalence relation splitting the infinite set of term orderings into a finite number of classes. Two orderings, τ_1 and τ_2 are equivalent with respect to an ideal I (and we shall say with respect to a design D) if and only if they have the same initial ideal

$$\text{Init}_{\tau_1}(I) = \langle \text{Lt}_{\tau_1}(g) : g \in G_{\tau_1} \rangle = \langle \text{Lt}_{\tau_2}(g) : g \in G_{\tau_2} \rangle = \text{Init}_{\tau_2}(I)$$

where G_{τ_j} is the Gröbner basis of I with respect to τ_j , $j = 1, 2$. This partition on the set of term orderings is called the *fan* of the ideal I , $\mathcal{F}(I)$ or $\mathcal{F}(D)$ when $I = I(D)$ for some design D . Each one of these equivalence classes is called a *leaf*. In particular leaves are characterised by initial ideals, that is τ_1 and τ_2 belong to the same leaf, L if and only if $\text{Init}_{\tau_1}(I) = \text{Init}_{\tau_2}(I)$. Moreover to each leaf L of the fan one can associate an order ideal E_L namely the set of terms which are not divisible by any of the elements in the corresponding initial ideal. When I is a design ideal $I(D)$ then E_L is finite and it is precisely $\text{Est}_{D,\tau}$ for all $\tau \in L$.

We define a N -point design in d dimensions to be maximal fan if it identifies all the models in d dimensions and with N terms that satisfy the divisibility condition that is that are order ideals. As an example, the design $D = \{(0, 0), (1, 1), (3, 2)\}$ is a *maximal fan* since it estimates all the two-dimensional models estimable by a three point design which are $\{1, x_1, x_1^2\}$, $\{1, x_1, x_2\}$ and $\{1, x_2, x_2^2\}$. A term ordering representative for the leaf $\{1, x_1, x_1^2\}$ is the lexicographic ordering with $x_2 > x_1$; for $\{1, x_1, x_2\}$ it is the tdeg ordering and for $\{1, x_2, x_2^2\}$ the lexicographic ordering with $x_1 > x_2$.

Ideally one would like to input all the information available on the term ordering before starting the computation, that is to define a pre-ordering on the variables instead of a term ordering. The computer algebra package CoCoA allows us to define a pre-ordering.

The algorithm to calculate fans of ideals takes a basis of the design ideal. At each step it chooses the possible leading terms compatible with the known ordering information, applies the S-polynomial test to check whether a set of polynomials is a Gröbner basis with respect to a given monomial ordering and keeps iterating to create new leaves of the fan. When the S-polynomial test is positive over one leaf it returns the Gröbner basis associated with that leaf and the conditions which the term orderings of that leaf must satisfy. This algorithm was first introduced in Mora and Robbiano (1988). The usual improvements to the Buchberger algorithm for reduced Gröbner bases can be applied.

Let us show the details with an example. Consider the design $D = \{(0,0), (1,2), (2,1)\}$ and impose the condition $x_1 > x_2$ on the term ordering. The design D is the set of solution of the following system of polynomial equations

$$\begin{aligned} f &= x_2^3 - 3x_2^2 + 2x_2 \\ g &= x_1 + 3/2x_2^2 - 7/2x_2. \end{aligned}$$

The possible leading terms of g (compatible with $x_1 > x_2$) are x_1 and x_2^2 , and for f we have only x_2^3 . We create two leaves in the fan $\mathcal{F}(D)$ characterised by the conditions $x_1 > x_2^2$ and $x_2^2 > x_1$ respectively. The S-polynomials are

$$\begin{aligned} S(f, g) &= -3x_2^2x_1 + 2x_1x_2 - 3/2x_2^5 + 7/2x_1^4 && \text{for } x_1 > x_2^2 \\ S(f, g) &= -\frac{2}{3}x_2^3 + 2x_2 - \frac{2}{3}x_2x_1 && \text{for } x_2^2 > x_1. \end{aligned}$$

Their remainders with respect to f and g are

$$\begin{aligned} p &= \text{Rem}(S(f, g), \{f, g\}) = 0 && \text{for } x_1 > x_2^2 \\ h &= \text{Rem}(S(f, g), \{f, g\}) = -\frac{2}{3}x_1x_2 + \frac{4}{9}x_1 + \frac{4}{9}x_2 && \text{for } x_2^2 > x_1. \end{aligned}$$

Since $p = 0$, by the S-polynomial test we have that for all the orderings such that $x_1 > x_2^2$ the set $\{f, g\}$ is a (reduced) Gröbner basis which gives $\{1, x_2, x_2^2\}$ as the estimable set.

We have to continue the calculation for the orderings such that $x_2^2 > x_1$. The new generating set is $\{f, g, h\}$ and the only possible leading term of h is x_1x_2 . Thus

$$\begin{aligned} S(f, h) &= -7/3x_1x_2^2 + 2x_1x_2 + 2/3x_2^3 \\ S(g, h) &= \frac{2}{3}(x_1^2 + x_2^2) - \frac{5}{3}x_1x_2 \end{aligned}$$

and

$$\begin{aligned} l &= \text{Rem}(S(f, h), \{f, g, h\}) = -14/9x_1^2 + 98/27x_1 - 28/27x_2 \\ m &= \text{Rem}(S(g, h), \{f, g, h\}) = \frac{2}{3}x_1^2 - \frac{14}{9}x_1 + \frac{4}{9}x_2. \end{aligned}$$

Because of the prior condition $x_1 > x_2$ on the ordering the only possible leading term of l and g is x_1^2 . The S-polynomial test shows that for the term orderings such that $x_2^2 > x_1$ and $x_1^2 > x_2$ the set $\{f, g, h, l, m\}$ is a Gröbner basis. The estimable set is $\{1, x_1, x_2\}$. In conclusion the fan of the design d with the constrained $x_1 > x_2$ is $\{\{1, x_2, x_2^2\}, \{1, x_1, x_2\}\}$.

If no condition on the ordering is imposed the above algorithm returns the fan of the ideal given as input. Alternatively to compute the fan one could use the so-called Gröbner walk techniques. A G-basis is computed with respect to some ordering, usually tdeg , and then from such basis the bases for the other blades are computed in a linear time. See Collart, Kalkbrener and Mall (1997)[21].

A design is called minimal fan when the fan of the design ideal has only one element. An interesting example is given by the class of full factorial designs. In general minimal fan designs are characterised by having a reduced total Gröbner basis whose leading terms are the same with respect to any term ordering. That is a total Gröbner basis.

Notice that also the Gröbner basis of the fraction of the full factorial including only points with at least one component assuming a specified value, let say $x_1 = a_1$

or $x_2 = a_2$ or ... $x_d = a_d$, is a total Gröbner basis. Indeed for a l^d -full factorial the Gröbner basis for the fraction described above is given by the set of polynomials describing the full factorial $P_i(\mathbf{x}) : i = 1, \dots, d$ (see Section 3.1.1) and the polynomial $(x_1 - a_1) \cdots (x_d - a_d)$. The leading terms of the P_i 's and of $(x_1 - a_1) \cdots (x_d - a_d)$ are the same with respect to any term ordering.

Caboara, Pistone, Riccomagno and Wynn (1997) [13] prove that echelon designs mentioned in Subsection 3.1.1 are also minimal fan designs. See also Robbiano and Rogantin (1997) [61]. In Subsection 3.3.1 we exploit the relation between fan of an ideal and polynomial interpolation.

3.3.1 Interpolation

For a particular design $D = \{x^{(1)}, \dots, x^{(N)}\}$ let E_L be the order ideal corresponding to a particular leaf L of the fan of D and let p_j for $j = 1, \dots, N$ be the elements of E_L , thus

$$E_L = \{p_1(x), \dots, p_N(x)\}.$$

Then the usual design matrix $X(E_L, D)$ for the model is

$$X(E_L, D) = \left\{ p_j(x^{(i)}) \right\}_{i,j=1}^N.$$

Since E_L is estimable the matrix $X(E_L, D)$ is invertible and equivalently $\det(X(E_L, D)) \neq 0$. Now the maximal set of leaves of dimension N subject to the (D) condition is well defined and finite. For $d = 2$ dimensions each such model can be mapped into a partition of N where the models (order ideals E_L) can be represented by solid dots on an integer grid. For example for $d = 2$, $N = 5$ the pattern

$$\begin{array}{c} \cdot \\ \cdot \\ \cdot \end{array}$$

corresponding to $5 = 2 + 2 + 1$ gives the model $1, x_1, x_1^2, x_2, x_1x_2$. One can check that there are 7 models hence the fan of a 5-point design in 2-dimension will have at most 7 leaves. This easily generalises to $d > 2$ using a generalised partition of integers.

Let $\mathcal{E}(D)$ be the set of models satisfying the (D) -condition and with N terms, where N is the size of the design D , and such that their design matrices at D are invertible. We say that the elements of $\mathcal{E}(D)$ are identifiable in a statistical sense. Let $\mathcal{F}(D)$ be the fan of the design D calculated as in Section 3.3. Elements of $\mathcal{F}(D)$ are algebraically identifiable. By Pistone and Wynn (1996) we have that algebraic identifiability implies statistical identifiability, that is $\mathcal{F}(D) \subseteq \mathcal{E}(D)$ and Caboara and Robbiano (1997) show with a counterexample that the inclusion may be strict: the model $E = \{1, x, x^2, y, y^2\}$ is statistically but not algebraically identifiable by the design $D = \{(0, 0), (0, -1), (1, 0), (1, 1), (-1, 1)\}$. However notice that the k -vector space generated by any model E in $\mathcal{E}(D)$ is isomorphic to the quotient $\mathbb{Q}[x]/I(d)$. For details see Pistone and Wynn (1996), Section 4. Theorem 16 below shows that subject to an additional condition to avoid designs and models in $\mathcal{E}(D) \setminus \mathcal{F}(D)$, there is a strong correspondence between interpolation and algebraic identifiability.

Let D be a N -point design and E an element of $\mathcal{E}(D)$. With an abuse of notation we list the terms of the saturated estimable model in a vector as follows

$$E(x) = (p_1(x), \dots, p_N(x))^t.$$

Suppose that the usual $N \times N$ design matrix

$$X = \{p_j(x^{(i)})\}_{i,j=1}^N$$

is invertible. We want to construct the initial ideal leading to E .

First we observe that given a term ordering every polynomial $f \in k[x]$ can be decomposed as a leading term $Lt(f, x) = Lt(f)$ and a tail $t(f, x) = Lt(f) - f$ in such a way that $f(x) = Lt(f, x) - t(f, x)$. Let G be a reduced G-basis. Then for all $h \in G$ none of the terms in $t(h, x)$ is divisible by any $Lt(g, x)$ for all $g \in G$. In other words for all $j = 1, \dots, J$ there exist a vector of length N with scalar entries, Θ_j such that the tail t_j is a linear combination of elements in $E(x)$

$$t_j(x) = E(x)^t \Theta_j$$

where J is the number of elements in G .

Next we observe that the complementary set of $E(x)$ in the set of all monomial terms in the variables x is a monomial ideal and thus by the Dickson's Lemma (see Little, Cox, O'Shea, 1992) we can construct a unique minimal finite basis of monomials of such a set. Let us denote such a basis by $Init = \{Lt_j(x)\}_{j=1}^J$. By construction the elements of $E(x)$ are those monomials not divisible by any of the $Lt_j(x)$, for $j = 1, \dots, J$. Indeed let x^α be an element of $E(x)$. By definition $x^\alpha \notin Init$. Let us suppose that x^α is divisible by one of the Lt_k for a k in $\{1, \dots, J\}$. Thus there exists a monomial x^β such that $x^\alpha = x^\beta Lt_k$, that is $x^\alpha \in \langle Lt_k \rangle \subset \langle Lt_j : j = 1, \dots, J \rangle = Init$. This is a contradiction and we are done.

Then we construct polynomials $t_j(x)$ which interpolate each of the terms in $Init$ using the model based on $E(x)$ at the design D , that is to say solve the following J linear systems of equations with respect to Θ_j

$$\begin{cases} Lt_j(x^{(1)}) = E(x^{(1)})^t \Theta_j = X \Theta_j \\ \vdots \\ Lt_j(x^{(N)}) = E(x^{(N)})^t \Theta_j = X \Theta_j. \end{cases}$$

Thus the t_j are uniquely determined because of the invertibility of X . Then define

$$g_j(x) = Lt_j(x) - t_j(x) \quad j = 1, \dots, J. \quad (3.2)$$

Now we are ready to state Theorem 16.

Theorem 16 *Let D be a design and E an element of $\mathcal{E}(D)$. Let $Init$ be constructed as above and let us suppose that there exists a term ordering τ such that $Lt_j(x)$ is the leading term of $g_j(x)$ with respect to τ for all $j = 1, \dots, J$. Then $E \in \mathcal{F}(D)$.*

Proof. The existence of τ follows by the fact that the hypothesis in the theorem defines the leading terms of the $g_j(x)$'s. That hypothesis is essential to avoid situations similar to the counterexample of Caboara and Robbiano (1997). We show

that the ideal generated by the $g_j(x)$'s namely $\langle g_j(x) \rangle$ is the design ideal, $I(D)$. Certainly by construction the design ideal includes the ideal generated by the g_j 's. Conversely let p be a polynomial in the design ideal and expand it in the g_j 's by the division algorithm using the term-ordering τ in the statement of the theorem:

$$p(x) = \sum_{j=1}^J s_j(x)g_j(x) + r(x).$$

Since $p(x)$ belongs to the design ideal and $g_j(x^{(i)}) = 0$ at all design points $x^{(i)}$ ($i = 1, \dots, N$) and for all $j = 1, \dots, J$ we have

$$p(x^{(i)}) = r(x^{(i)}) = 0.$$

Now the division algorithm always yields a remainder $r(x)$ every monomial of which is dominated by the leading terms of the $g_j(x)$, in this case the $Lt_j(x)$. But by the assumption in the theorem the monomials must be from $E(x)$. Since the design matrix for $E(x)$ at the design d is invertible, then $r(x) = 0$ identically. This implies that $p(x) \in \langle g_j(x) \rangle$.

Finally we show that the set $G = \{g_j(x) : j = 1, \dots, J\}$ is a (reduced) G-basis for the design ideal. We use the S-polynomial test. Consider a generic S-polynomial and proceed as above by expanding it on G

$$S(g_l, g_k) = \sum_{j=1}^J s_j(x)g_j(x) + r(x)$$

and by evaluating it at the design points. Since $S(g_l, g_k) \in \langle g_j(x) : j = 1, \dots, J \rangle$, it must be zero at the design points leading to $r(x^{(i)}) = 0$ for all design points. But again since $r(x)$ is a linear combination of elements in $E(x)$ which is estimable we must have $r(x) = 0$ identically. Notice that by construction $\{g_j(x) : j = 1, \dots, J\}$ is reduced. ■

The following example clarifies the three steps of the proof. Consider the two-dimensional design $D = \{(0,0), (1,0), (0,1), (2,1)\}$ and the estimable model $E = \{1, x_1, x_2, x_1^2\}$. We check estimability simply by checking that the design matrix

$$X = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 2 & 1 & 4 \end{pmatrix}$$

is invertible. The set of leading terms giving E is $Init = \{x_1^3, x_1x_2, x_2^2\} = \{Lt_1(x), Lt_2(x), Lt_3(x)\}$. Note that the condition in Theorem 16 is satisfied. We have the interpolators of the elements of $Init$

$$\begin{cases} t_1(x) = 3x_1^2 - 2x_1 \\ t_2(x) = x_1^2 - x_1 \\ t_3(x) = x_2. \end{cases}$$

Thus the Gröbner basis is

$$\begin{cases} g_1(x) = x_1^3 - 3x_1^2 + 2x_1 \\ g_2(x) = x_1x_2 - x_1^2 + x_1 \\ g_3(x) = x_2^2 - x_2. \end{cases}$$

The leading term of g_2 must be x_1x_2 and thus we require that $x_1x_2 > x_1^2$ which implies that the term orderings such that $x_2 > x_1$ belong to the leaf of $E(x)$.

For the counterexample mentioned above the set of interpolating polynomials is as follows

$$\begin{cases} xy &= -x^2 + y^2/2 + x + y/2 \\ x^3 &= x \\ y^3 &= y. \end{cases}$$

The condition in Theorem 16 is not met since there does not exist a term ordering such that xy is leading term of the first polynomial. Indeed it should simultaneously be $xy > x^2$ and $xy > y^2$, that is $y > x$ and $x > y$ which is not possible in a total ordering.

3.4 The model ideal

In this section we develop the notion of interpolation in a rather more conventional form introducing the model ideal and the experiment ideal. Let us consider the linear polynomial models and write for example the quadratic model

$$y = \theta_0 + \theta_1x + \theta_2x^2$$

in the form

$$y - \theta_0 - \theta_1x - \theta_2x^2 = 0.$$

This is a polynomial variety V in $\mathbb{Q}(\theta_0, \theta_1, \theta_2)[x, y]$ and has a natural ideal: the ideal of all polynomials which also have zeros at the model/variety's zeros.

Notice immediately that we can generalise to a polynomial in x, θ and y . Using a notation which allows also multivariate x, θ and y we can write the model ideal as generated by

$$q(y, \theta, x).$$

In system terms we think of

$$\begin{aligned} y &: \text{observations (output)} \\ \theta &: \text{unobservable (state parameters)} \\ x &: \text{inputs (design variables)}. \end{aligned}$$

Now suppose that we conduct an experiment consisting of observing Y_i at the design points x_i , for $i = 1, \dots, N$. That is we have a set of pairs

$$(x_1, Y_1), \dots, (x_N, Y_N) \in \text{Design Space} \times \text{Observation Space}.$$

Consider the above quadratic model and assume that $N = 2$. We know that θ_0 , θ_1 and θ_2 are not all identifiable given $(x_1, Y_1), (x_2, Y_2)$ because the model is over specified. The question arises: what is identifiable?

The identifiability problem is solved nicely in the following manner. We generalise the idea of a design ideal to include the observations Y_1, \dots, Y_N . Let y be the indeterminate representing the observations. We shall call this the *experiment ideal*. We do this by simply setting up a design ideal in the (x, y) space forgetting (mathematically) that x is controlled and y is observed. In the quadratic example we have the ideal for the two points $(x_1, Y_1), (x_2, Y_2)$ in two dimensions.

The procedure is to factor the experiment ideal into the model ideal leading to a remainder of the form

$$\sum_{\alpha} h_{\alpha} z^{\alpha}$$

where $z = (x, y)$ and the h_{α} are function of θ and $(x_1, Y_1), \dots, (x_N, Y_N)$. It is basic that at the pairs (x_i, Y_i) the remainder is zero. Now given an actual design (x_1, \dots, x_N) we can consider the h_{α} as functions of $Y_D = (Y_1, \dots, Y_N)$ and write $h_{\alpha}(\theta, Y_D)$.

Starting with a particular term ordering the independence of the “residual” vector space spanned by $\{z^{\alpha}\}$ in the remainder requires that

$$h_{\alpha}(\theta, Y_D) = 0 \quad \text{for all } \alpha \text{ in the residual.}$$

These conditions give the *confounding* structure. The model is fully identifiable by the given design if and only if these equations give a unique solution of θ as function of Y_D .

Suppose in the quadratic model above we take $N = 2$ and $x_1 = -1, x_2 = 1$. Then the experiment ideal for the points $(-1, Y_1)$ and $(1, Y_2)$ has the following Gröbner basis with respect to $\text{plex}(y > x)$

```
> DesObs:=[t[1]*(x-1),t[1]*(y-Y[1]),t[2]*(x+1),t[2]*(y-Y[2]),t[1]+t[2]-1]:
```

```
> DesObs:=gbasis(DesObs, [t[1],t[2],y,x], plex):
```

```
> DesObs:=[ seq(DesObs[k], k=3..nops(DesObs) )];
```

$$\text{DesObs} := [-Y_1 - Y_2 + (-Y_1 + Y_2)x + 2y, -1 + x^2]$$

```
> Model:=y-theta[2]*x^2-theta[1]*x-theta[0]:
```

```
> REM:=normalf(Model, DesObs, [y,x]):
```

$$\text{REM} := -\theta_0 - \theta_2 + \frac{1}{2}Y_1 + \frac{1}{2}Y_2 + \left(\frac{1}{2}Y_1 - \frac{1}{2}Y_2 - \theta_1\right)x$$

```
> hh:=coeffs(REM,[y,x]): h[1]:=hh[1]; h[2]:=hh[2];
```

$$h_1 := -\theta_0 - \theta_2 + \frac{1}{2}Y_1 + \frac{1}{2}Y_2$$

$$h_2 := \frac{1}{2}Y_1 - \frac{1}{2}Y_2 - \theta_1$$

We solve $h_1 = h_2 = 0$ and find that θ_1 is identifiable and only a linear function of θ_2 and θ_0 is identifiable

$$\theta_1 = \frac{1}{2}(Y_1 - Y_2)$$

$$\theta_2 + \theta_0 = \frac{1}{2}(Y_1 - Y_2).$$

By considering the ordering $\text{plex}(x > y)$ we find

$$h_1 := -\frac{\theta_0 Y_1 - \theta_1 Y_1 + \theta_2 Y_1 - \theta_0 Y_2 - \theta_2 Y_2 - \theta_1 Y_2}{Y_1 - Y_2}$$

$$h_2 := -\frac{-Y_1 + Y_2 + 2\theta_1}{Y_1 - Y_2}$$

which gives the same result as above

$$\begin{aligned}\theta_1 &= \frac{1}{2}(Y_1 - Y_2) \\ \theta_2 + \theta_0 &= \frac{1}{2}(Y_1 - Y_2)\end{aligned}$$

but with the additional condition $Y_1 \neq Y_2$. The same result is obtained using the term orderings $\text{tdeg}(x > y)$ and $\text{tdeg}(y > x)$.

The independence of the solution from the term ordering is not guaranteed in general (see Section 3.3). But notice that for models linear in the parameters θ 's the h 's are linear in the θ 's because the division operates linearly on the coefficients of the dividend. This in particular implies that for all term orderings the same h 's are obtained apart from a multiplicative constant. Indeed let us consider an experiment ideal I in $k[x, y]$ and two different term-orderings τ_1 and τ_2 . Let G_1 and G_2 be the Gröbner bases of I with respect to τ_1 and τ_2 and finally let B_1 and B_2 be the set of monomials spanning the remainder sets obtained when dividing by G_1 and G_2 respectively. It is known that there exists a k -vector space isomorphism between the vector spaces generated by G_1 and G_2 . Thus there is a non-singular linear mapping from the h 's calculated with respect to τ_1 and the h 's calculated with respect to τ_2 and thus the conditions $h = 0$ must lead to the same solution for the θ 's.

It is interesting to observe what happens when we have more observations than required to fit the model. For example consider the model

$$y = \theta x$$

that is

$$g(y, \theta, x) = y - \theta x$$

and take the two (x, y) points $(1, Y_1)$ and $(2, Y_2)$. Considering $y > x$ and the lex ordering the Gröbner basis for the design is

$$\{-2Y_1 + Y_2 + (Y_1 - Y_2)x + y, 2 - 3x + x^2\}$$

which leads to the vector-space basis $1, x$. The remainder is

$$2Y_1 - Y_2 + (-\theta - Y_1 + Y_2)x$$

giving $\theta = Y_2 - Y_1$ and $2Y_1 - Y_2 = 0$. It is important to note that although we seem to have started with arbitrary Y_1 and Y_2 the remainder gives us back the required condition on the data Y_1, Y_2 forced by the model, that is $y = px$ implies $Y_1 = pY_2$ for all p constants.

Here is a more complex example in which y appears implicitly in the model. Starting with the inverse polynomial model

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \frac{\theta_3}{x_1 x_2}$$

we obtain (ignoring $x_1 = 0$ and $x_2 = 0$)

$$y x_1 x_2 - \theta_0 x_1 x_2 - \theta_1 x_1^2 x_2 - \theta_2 x_1 x_2^2 - \theta_3 = 0.$$

Now we consider $N = 3$ and the three points (x_1, x_2) , $(1, 1)$, $(2, 1)$ and $(1, 2)$. Since the model is linear in the parameters θ 's we chose arbitrarily the term ordering lex and obtain the following Gröbner basis for the experimental ideal

$$\text{DesGB} := [y + (Y_1 - Y_2)x_1 - 3Y_1 + Y_2 + Y_3 + (Y_1 - Y_3)x_2, \\ x_1^2 - 3x_1 + 2, x_1x_2 - x_1 + 1 - x_2, 2 - 3x_2 + x_2^2]$$

The division of the model with respect to the above Gröbner basis returns

$$\text{Resto} := (-\theta_0 + 2Y_2 - 3\theta_1 - \theta_2 - Y_1)x_1 + (-\theta_1 - Y_1 + 2Y_3 - \theta_0 - 3\theta_2)x_2 \\ - \theta_3 + \theta_0 - 2Y_2 + 3\theta_1 + 3\theta_2 + 3Y_1 - 2Y_3$$

and we obtain the following system of linear equations in the θ 's

$$h_1 := -\theta_3 + \theta_0 - 2Y_2 + 3\theta_1 + 3\theta_2 + 3Y_1 - 2Y_3$$

$$h_2 := -\theta_0 + 2Y_2 - 3\theta_1 - \theta_2 - Y_1$$

$$h_3 := -\theta_1 - Y_1 + 2Y_3 - \theta_0 - 3\theta_2$$

Equating the coefficients to zero we have

$$\theta_0 + 4\theta_2 = -Y_1 - Y_2 + 3Y_3$$

$$\theta_1 - \theta_2 = -Y_3 + Y_2$$

$$\theta_3 - 2\theta_2 = 2Y_1 - 2Y_3.$$

We now consider a genuinely non-linear model which can be turned into a model in which y is included implicitly

$$> \text{LogModel} := y - \theta_0 - \frac{\theta_1}{1 + \theta_2 x_1} - \frac{\theta_3}{1 + \theta_4 x_2};$$

$$\text{LogModel} := y - \theta_0 - \frac{\theta_1}{1 + \theta_2 x_1} - \frac{\theta_3}{1 + \theta_4 x_2}$$

giving

$$> \text{LogModel0} := \text{simplify}((1 + \theta_2 x_1) * (1 + \theta_4 x_2) * \text{LogModel});$$

$$\text{LogModel0} := y + y\theta_4 x_2 + y\theta_2 x_1 + y\theta_2 x_1 \theta_4 x_2 - \theta_0 - \theta_0 \theta_4 x_2 \\ - \theta_0 \theta_2 x_1 - \theta_0 \theta_2 x_1 \theta_4 x_2 - \theta_1 - \theta_1 \theta_4 x_2 - \theta_3 - \theta_3 \theta_2 x_1$$

At the 2^2 -full factorial design we make the observation Y_1, Y_2, Y_3, Y_4 and get the following Gröbner basis with respect to the term ordering $\text{lex}(y > x_1 > x_2)$

$$\text{DesGB} := [4y + (-Y_1 + Y_3 + Y_2 - Y_4)x_1x_2 - Y_1 - Y_3 - Y_4 - Y_2 \\ + (-Y_1 - Y_3 + Y_2 + Y_4)x_2 + (-Y_1 + Y_3 + Y_4 - Y_2)x_1, x_1^2 - 1, -1 + x_2^2]$$

Equating to zero the coefficients of the remainder of LogModel0 by the Gröbner basis we get the following system of four equations in five unknown θ 's

$$> \mathbf{A} := [\text{coeffs}(\text{Resto}, [y, x[1], x[2]])];$$

$$> \mathbf{h}[1] := \mathbf{A}[1]; \mathbf{h}[2] := \mathbf{A}[2]; \mathbf{h}[3] := \mathbf{A}[3]; \mathbf{h}[4] := \mathbf{A}[4];$$

$$h_1 := -\theta_0 - \theta_1 - \theta_3 + \frac{1}{4}Y_1 + \frac{1}{4}Y_3 + \frac{1}{4}Y_4 + \frac{1}{4}Y_2 + \frac{1}{4}\theta_2 Y_1 - \frac{1}{4}\theta_2 Y_3 - \frac{1}{4}\theta_2 Y_4 \\ + \frac{1}{4}\theta_2 Y_2 + \frac{1}{4}Y_1 \theta_4 + \frac{1}{4}Y_3 \theta_4 - \frac{1}{4}Y_2 \theta_4 - \frac{1}{4}Y_4 \theta_4 + \frac{1}{4}\theta_2 \theta_4 Y_1 \\ - \frac{1}{4}\theta_2 \theta_4 Y_3 - \frac{1}{4}\theta_2 \theta_4 Y_2 + \frac{1}{4}\theta_2 \theta_4 Y_4$$

$$\begin{aligned}
h_2 := & \frac{1}{4} Y_4 \theta_4 + \frac{1}{4} Y_3 \theta_4 - \theta_0 \theta_4 + \frac{1}{4} Y_2 \theta_4 - \theta_1 \theta_4 + \frac{1}{4} Y_1 \theta_4 + \frac{1}{4} Y_1 + \frac{1}{4} Y_3 \\
& - \frac{1}{4} Y_2 - \frac{1}{4} Y_4 + \frac{1}{4} \theta_2 \theta_4 Y_1 - \frac{1}{4} \theta_2 \theta_4 Y_3 - \frac{1}{4} \theta_2 \theta_4 Y_4 + \frac{1}{4} \theta_2 \theta_4 Y_2 \\
& + \frac{1}{4} \theta_2 Y_1 - \frac{1}{4} \theta_2 Y_3 - \frac{1}{4} \theta_2 Y_2 + \frac{1}{4} \theta_2 Y_4
\end{aligned}$$

$$\begin{aligned}
h_3 := & -\theta_0 \theta_2 - \theta_3 \theta_2 + \frac{1}{4} \theta_2 Y_1 + \frac{1}{4} \theta_2 Y_3 + \frac{1}{4} \theta_2 Y_4 + \frac{1}{4} \theta_2 Y_2 + \frac{1}{4} Y_1 - \frac{1}{4} Y_3 \\
& - \frac{1}{4} Y_4 + \frac{1}{4} Y_2 + \frac{1}{4} \theta_2 \theta_4 Y_1 + \frac{1}{4} \theta_2 \theta_4 Y_3 - \frac{1}{4} \theta_2 \theta_4 Y_2 - \frac{1}{4} \theta_2 \theta_4 Y_4 \\
& - \frac{1}{4} Y_3 \theta_4 + \frac{1}{4} Y_1 \theta_4 - \frac{1}{4} Y_2 \theta_4 + \frac{1}{4} Y_4 \theta_4
\end{aligned}$$

$$\begin{aligned}
h_4 := & -\theta_0 \theta_2 \theta_4 + \frac{1}{4} \theta_2 \theta_4 Y_1 + \frac{1}{4} \theta_2 \theta_4 Y_3 + \frac{1}{4} \theta_2 \theta_4 Y_4 + \frac{1}{4} \theta_2 \theta_4 Y_2 + \frac{1}{4} \theta_2 Y_1 \\
& + \frac{1}{4} \theta_2 Y_3 - \frac{1}{4} \theta_2 Y_2 - \frac{1}{4} \theta_2 Y_4 + \frac{1}{4} Y_1 \theta_4 - \frac{1}{4} Y_3 \theta_4 - \frac{1}{4} Y_4 \theta_4 + \frac{1}{4} Y_2 \theta_4 \\
& - \frac{1}{4} Y_3 + \frac{1}{4} Y_1 - \frac{1}{4} Y_2 + \frac{1}{4} Y_4
\end{aligned}$$

The above system has the following four sets of solutions

> `gsolve({h[1],h[2],h[3],h[4]},{theta[0],theta[1],theta[2],theta[3],theta[4]});`

$$\begin{aligned}
& \left[\left[2\theta_1 + 2\theta_0 - Y_1 - Y_3 + (-Y_1 + Y_3)\theta_2, \theta_3, \right. \right. \\
& \quad \left. \left. 2\theta_0\theta_2 - Y_1 + Y_3 + (-Y_1 - Y_3)\theta_2, \theta_4 - 1 \right], \left[\right. \right. \\
& \quad \left. \left. 2\theta_1 + 2\theta_0 - Y_4 - Y_2 + (Y_4 - Y_2)\theta_2, \theta_3, \right. \right. \\
& \quad \left. \left. 2\theta_0\theta_2 + Y_4 - Y_2 + (-Y_4 - Y_2)\theta_2, \theta_4 + 1 \right], \left[\theta_1, \right. \right. \\
& \quad \left. \left. 2\theta_0 - Y_1 - Y_2 + (-Y_1 + Y_2)\theta_4 + 2\theta_3, \right. \right. \\
& \quad \left. \left. 2\theta_0\theta_4 - Y_1 + Y_2 + (-Y_1 - Y_2)\theta_4, \theta_2 - 1 \right], \left[\theta_1, \right. \right. \\
& \quad \left. \left. 2\theta_0 - Y_3 - Y_4 + (-Y_3 + Y_4)\theta_4 + 2\theta_3, \right. \right. \\
& \quad \left. \left. 2\theta_0\theta_4 - Y_3 + Y_4 + (-Y_3 - Y_4)\theta_4, \theta_2 + 1 \right] \right]
\end{aligned}$$

None of the above four solutions is acceptable since they would annihilate the denominator. Indeed by direct computation we obtain the following system of equations that admits no solution in the θ 's for generic Y_i 's ($i = 1, \dots, 4$)

$$\begin{cases} Y_1 = \theta_0 + \frac{\theta_1}{1+\theta_2} + \frac{\theta_3}{1+\theta_4} \\ Y_2 = \theta_0 + \frac{\theta_1}{1+\theta_2} + \frac{\theta_3}{1-\theta_4} \\ Y_3 = \theta_0 + \frac{\theta_1}{1-\theta_2} + \frac{\theta_3}{1+\theta_4} \\ Y_4 = \theta_0 + \frac{\theta_1}{1-\theta_2} + \frac{\theta_3}{1-\theta_4} \end{cases}$$

since for all θ_0 it is equivalent to the system

$$\begin{cases} Y_1 - Y_2 = \theta_3 \left(\frac{1}{1+\theta_4} - 1 \frac{1}{1-\theta_4} \right) \\ Y_3 - Y_4 = \theta_3 \left(\frac{1}{1+\theta_4} - 1 \frac{1}{1-\theta_4} \right) \\ Y_1 - Y_3 = \theta_1 \left(\frac{1}{1+\theta_2} - 1 \frac{1}{1-\theta_2} \right) \\ Y_2 - Y_4 = \theta_2 \left(\frac{1}{1+\theta_2} - 1 \frac{1}{1-\theta_2} \right) \end{cases}$$

which gives $\frac{Y_1 - Y_2}{Y_3 - Y_4} = 1 = \frac{Y_1 - Y_3}{Y_2 - Y_4}$ and thus imposes constraints on the observations. The same as above happens when the design is a generic dilation of the standard 2^2 -full factorial given by $(\pm N, \pm N)$ for any N constant. For the design $\{(2, 2), (1, -1), (-1, 1), (1, 1)\}$ we get the following admissible solution

$$\begin{aligned} \theta_1 &= \frac{1}{2} \frac{Y_1 \theta_2^2 - \theta_2^2 Y_3 + Y_3 - Y_1}{\theta_2} \\ \theta_2 &= \theta_2 \\ \theta_3 &= \frac{3}{2} (Y_1 - Y_2) \frac{(-3Y_3 + 3Y_3 \theta_2 + Y_1 + Y_1 \theta_2 + 2Y_4 - 4Y_4 \theta_2)}{(4Y_1 \theta_2 - 6Y_2 \theta_2 - 6Y_3 \theta_2 + 8Y_4 \theta_2 + 6Y_3 - 5Y_1 + 3Y_2 - 4Y_4)} \\ &\quad \frac{(3Y_1 \theta_2 - 3Y_3 \theta_2 - 4Y_2 \theta_2 + 4Y_4 \theta_2 - 3Y_1 + 3Y_3 - 2Y_4 + 2Y_2)}{(3Y_3 - 2Y_4 + 3Y_2 + 4Y_4 \theta_2 + 5Y_1 \theta_2 - 6Y_2 \theta_2 - 3Y_3 \theta_2 - 4Y_1)} \\ \theta_4 &= \frac{1}{2} \frac{(8Y_1 Y_4 - 5Y_2 Y_1 - Y_1 Y_3 - 4Y_2 Y_4 - 3Y_2 Y_3 + 4Y_3 Y_4 + 4Y_1^2 - 3Y_3^2) \theta_2^2}{((5Y_1 - 6Y_2 - 3Y_3 + 4Y_4) \theta_2 - 4Y_1 + 3Y_3 - 2Y_4 + 3Y_2) \theta_2} \\ &\quad + \frac{1}{2} \frac{(-2Y_2 Y_1 - 6Y_3 Y_4 - 6Y_1 Y_3 + 6Y_2 Y_3 + 2Y_2 Y_4 + 6Y_3^2) \theta_2}{((5Y_1 - 6Y_2 - 3Y_3 + 4Y_4) \theta_2 - 4Y_1 + 3Y_3 - 2Y_4 + 3Y_2) \theta_2} \\ &\quad + \frac{1}{2} \frac{+7Y_1 Y_3 + 3Y_2 Y_1 - 3Y_2 Y_3 - 4Y_1^2 - 2Y_1 Y_4 - 3Y_3^2 + 2Y_3 Y_4}{((5Y_1 - 6Y_2 - 3Y_3 + 4Y_4) \theta_2 - 4Y_1 + 3Y_3 - 2Y_4 + 3Y_2) \theta_2} \end{aligned}$$

for all $\theta_2 \notin \left\{ 0, \frac{4Y_1 - 3Y_3 + 2Y_4 - 3Y_2}{5Y_1 - 6Y_2 - 3Y_3 + 4Y_4}, \frac{5Y_1 - 3Y_2 - 6Y_3 + 4Y_4}{2(2Y_1 - 3Y_2 - 3Y_3 + 4Y_4)} \right\}$.

Summary

In this chapter we present the novel use of algebraic geometry in the design of experiments. The starting point is to express an experimental design as the solution of polynomial equations, namely an algebraic variety. From this we obtain the corresponding polynomial ideal. The basic theory is exposed in detail: the construction of the design ideal given the design points and the algorithm to determine a saturated set of identifiable polynomial terms are discussed. The theory relies heavily on Gröbner bases and is an alternative to the classical approach to experimental design in terms of groups and allows us to consider designs with any structure. The classical concept of aliasing find a nice interpretation and extension in this new approach. Many examples are considered.

Particular attention is given to the connection between the procedure exposed and the concept of interpolation. This lead to the notion of the fan of a design, that is the class of models obtainable using the Gröbner basis method, and in particular of maximal and minimal fan. Finally the same algebraic procedure is applied to the model ideal so that non-linear models can be considered within this framework.

Part II

**Fourier Models and Lattice
Designs**

Chapter 4

Generalities for Fourier models and lattice grids

In this part of the thesis we show that some orthogonal designs for Fourier models are in the class of uniform designs based on one-generator lattice grids: we refer to designs based on lattice grids as lattice designs. In this chapter we define Fourier models, state some of their properties and discuss their place in the literature, particularly Engineering literature where their analogue is the discrete Fourier transform. Some well known facts on D -optimal designs are reported in order to establish the background to the problem. A dictionary of examples of Fourier model types follows. The second part of this chapter defines lattice designs, their basic properties and their use in integration.

4.1 Fourier models

Definition 21 Let $A^+ \subset \mathbb{Z}^d$ be a set of integer vectors such that

- (i) $0 \notin A^+$,
- (ii) if $h \in A^+$ then $-h \notin A^+$,
- (iii) A^+ is finite that is $\#(A^+) < \aleph_0$.

Also define $A := A^+ \cup \{-A^+\} \cup \{0\}$ and let $\#(A) = 2m + 1$.

Although the results have general applicability we shall refer to the vectors in A as *frequencies*. The set A will index the set of parameters according to the following definition.

Definition 22 Through A we define the following trigonometric regression model or Fourier model

$$\begin{aligned} E(Y(x)) &= \theta_0 + \sqrt{2} \sum_{h \in A^+} [\theta_h \sin(2\pi h^t x) + \phi_h \cos(2\pi h^t x)] \\ &= \alpha_0 + \sum_{h \in A^+} [\beta_h e^{2\pi i h^t x} + \delta_h e^{-2\pi i h^t x}] \end{aligned}$$

where $x \in [0, 1]^d$, $\theta_0, \theta_h, \phi_h \in \mathbb{R}$ and $\alpha_0, \beta_h, \delta_h \in \mathbb{C}$ are related as follows

$$\begin{aligned}\alpha_0 &= \theta_0 \\ \beta_h &= \frac{\phi_h - i\theta_h}{\sqrt{2}} \\ \delta_h &= \frac{\phi_h + i\theta_h}{\sqrt{2}}.\end{aligned}$$

The model can be expressed in more compact form as

$$E(Y(x)) = \sum_{h \in A} e^{2\pi i h^t x}$$

but we prefer to decompose it over A^+ as a constant term (α_0), a sum over A^+ of sine terms ($+h$) and a sum over A^+ of cosine terms ($-h$). Moreover note that the set A , that uniquely determines the model, may be generated by more than one set A^+ , but that any set A^+ defining A is a subset of A itself. The notation A^+ denotes our preference for frequencies whose components are all positive integer numbers.

Fourier models assume real values but we also consider the complex representation; see Kobilinsky (1990) [41] for a deeper insight on the group nature of Fourier models. The two forms of the model, real and complex, can be written in matrix form as

$$E(Y(x)) = X(x) \theta = Z(x) \alpha$$

where the parameter and regression vectors are as follows

$$\begin{aligned}\theta &= (\theta_0 : (\theta_h)_{h \in A^+} : (\phi_h)_{h \in A^+})^t \\ X(x) &= (1 : (\sqrt{2} \sin(2\pi h^t x))_{h \in A^+} : (\sqrt{2} \cos(2\pi h^t x))_{h \in A^+}) \\ \alpha &= (\alpha_0 : (\beta_h)_{h \in A^+} : (\delta_h)_{h \in A^+})^t \\ Z(x) &= (1 : (e^{2\pi i h^t x})_{h \in A^+} : (e^{-2\pi i h^t x})_{h \in A^+}).\end{aligned}$$

Fourier models are one-periodic in each dimension and periodicity enables us to extend them to \mathbb{R}^d with infinite regularity. In this part of the thesis the design region for Fourier models will always be the unitary hypercube $[0, 1]^d$ thus $E(Y(0)) = E(Y(1))$ and only one of the x -value is included. On the one hand the periodicity makes Fourier models ideal for studying periodic phenomena, on the other hand it may seem a restriction. One can try to avoid this restriction by enlarging, shifting, or randomising the design. Also there are methods for periodising non-periodic functions, see Sloan and Joe (1994) [69].

For applications of Fourier models we refer to the extensive engineering literature. To estimate the parameters the classical approach in that field is to consider the sets $\{\sqrt{2} \sin(2\pi h^t x), \sqrt{2} \cos(2\pi h^t x) : h \in A^+\}$ and $\{e^{2\pi i h^t x}, e^{-2\pi i h^t x} : h \in A^+\}$ of orthogonal functions on $[0, 1]^d$ with respect to the Lebesgue measure. From the standard Fourier theory multiplying the equality

$$E(Y(x)) = \theta_0 + \sqrt{2} \sum_{h \in A^+} [\theta_h \sin(2\pi h^t x) + \phi_h \cos(2\pi h^t x)]$$

by $\sqrt{2} \sin(2\pi h_0^t x)$ or $\sqrt{2} \cos(2\pi h_0^t x)$, for $h_0 \in A$, and integrating over $[0, 1]^d$ one has

$$\begin{aligned}\theta_{h_0} &= \int_{[0,1]^d} \sqrt{2} \sin(2\pi h_0^t x) E(Y(x)) dx \\ \text{or } \phi_{h_0} &= \int_{[0,1]^d} \sqrt{2} \cos(2\pi h_0^t x) E(Y(x)) dx\end{aligned}$$

and simply

$$\alpha_0 = \theta_0 = \int_{[0,1]^d} E(Y(x)) dx.$$

Alternatively working directly with the complex representation then multiplying by $e^{-2\pi i h_0^t x}$ or $e^{2\pi i h_0^t x}$ one finds

$$\begin{aligned}\beta_{h_0} &= \int_{[0,1]^d} e^{-2\pi i h_0^t x} E(Y(x)) dx \\ \text{or } \delta_{h_0} &= \int_{[0,1]^d} e^{2\pi i h_0^t x} E(Y(x)) dx.\end{aligned}$$

Instead of evaluating and approximating these integrals we approach the problem of estimation and identification of the parameters via the theory of experimental design. We redefine a design in order to allow replications.

Definition 23 We define a design $D = \{x_1, \dots, x_N\}$, $N \in \mathbb{Z}_+^*$ to be a finite set of not necessarily distinct points in $[0, 1]^d$. The matrices

$$X = \begin{pmatrix} X(x_1) \\ \vdots \\ X(x_N) \end{pmatrix} \quad \text{and} \quad Z = \begin{pmatrix} Z(x_1) \\ \vdots \\ Z(x_N) \end{pmatrix}$$

are called the real and complex design matrix.

Let $Y_i = E(Y(x_i))$ be the observed value at the design point x_i , $i = 1, \dots, N$ and $Y = (Y_1, \dots, Y_N)^t$ the observed vector. For sake of example we assume a real design matrix. In compact form we write

$$Y = X\theta$$

and multiplying this equality by X^t we obtain

$$X^t Y = X^t X \theta.$$

The matrix $X^t X$ is called the information matrix. Now we assume that $X^t X$ is invertible, that is X is full rank, and obtain

$$\theta = (X^t X)^{-1} X^t Y.$$

We suppose that

$$Y(x) = E(Y(x)), \quad Y_i = E(Y(x_i))$$

are the expected model values of the regression statistical model

$$Y(x) = E(Y(x)) + \epsilon, \quad Y_i = E(Y(x_i)) + \epsilon_i \quad (i = 1, \dots, N)$$

where ϵ follows a normal $\mathcal{N}(0, \sigma^2)$ distribution with $0 < \sigma^2 < +\infty$ and the ϵ_i 's are uncorrelated errors with zero mean and equal variance, σ^2 . Assuming X has full rank, by the Gauss-Markov theorem the least squares estimator

$$\hat{\theta} = (X^t X)^{-1} X^t Y$$

is the best linear unbiased estimator of θ .

Definition 24 A design such that $X^t X = NI$ is said to be orthogonal with respect to the model.

Thus for an orthogonal design, the following vector

$$\hat{\theta} = \frac{1}{N} X^t Y$$

estimates θ as the weighted mean of the observed values at the design points.

Next we show how the orthogonality condition $X^t X = NI$ translates to the complex form before summarizing the optimum design theory of experimental design and presenting the classes of Fourier models we use extensively.

The equation relating α and θ is

$$\alpha = H\theta$$

where H is given by

$$H = \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & -\frac{i}{\sqrt{2}}I & \frac{1}{\sqrt{2}}I \\ \hline 0 & \frac{i}{\sqrt{2}}I & \frac{1}{\sqrt{2}}I \end{array} \right).$$

The symbol I denotes the $m \times m$ identity matrix. Note that H is an unitary matrix that is $H^* H = I$ equivalently $H^{-1} = H^*$, where H^* is the conjugate transpose matrix of H . We have

$$E(Y(x)) = X\theta = XH^{-1}H\theta = XH^{-1}\alpha = Z\alpha$$

where $Z = XH^{-1}$ is actually the complex design matrix.

Theorem 17 The best linear unbiased estimator for θ provides the corresponding estimator for α ,

$$\hat{\alpha} = H\hat{\theta}.$$

Proof. Let Z^* be the transpose and conjugate matrix of Z in particular $Z^* = (XH^{-1})^* = HX^t$. By straightforward calculation we have

$$\begin{aligned} \hat{\alpha} &= (Z^* Z)^{-1} Z^* Y \\ &= (HX^t XH^{-1})^{-1} HX^t Y \\ &= H(X^t X)^{-1} X^t Y \\ &= H\hat{\theta}. \quad \blacksquare \end{aligned}$$

The next theorem translates the orthogonality condition on the complex design matrix.

Theorem 18 *Given a design with N points and a Fourier model with regression vector $X(x)$ in real form and $Z(x)$ in complex form, the orthogonality condition $X^t X = NI$ holds if and only if $Z^* Z = NI$ holds.*

Proof. From the definitions we have the following $Z^* Z = H X^t X H^{-1}$ and $X^t X = H^{-1} Z^* Z H$. ■

The matrix $Z^* Z$ has the following block structure

$$Z^* Z = \begin{pmatrix} N & a_1 & b_1 \\ a_2 & A & C \\ b_2 & D & B \end{pmatrix}$$

where for all $h_1, h_2 \in A^+$

$$\begin{aligned} a_{1h_1} &= b_{2h_1} &= \sum_{x \in D} e^{2\pi i h_1^t x} \\ a_{2h_1} &= b_{1h_1} &= \sum_{x \in D} e^{-2\pi i h_1^t x} \\ A_{h_1, h_2} &= \sum_{x \in D} e^{2\pi i (-h_1 + h_2)^t x} \\ C_{h_1, h_2} &= \sum_{x \in D} e^{2\pi i (-h_1 - h_2)^t x} \\ D_{h_1, h_2} &= \sum_{x \in D} e^{2\pi i (+h_1 + h_2)^t x} \\ B_{h_1, h_2} &= \sum_{x \in D} e^{2\pi i (+h_1 - h_2)^t x} \end{aligned} \tag{4.1}$$

and $a_1 = a_2^t = b_2^t = b_1^*$, $A = B^*$ and $C = D^*$. The conditions for orthogonality are, then, $a_1 = a_2^t = b_2^t = b_1^* = 0$, $C = D = 0$ and $A = B = NI$. On the diagonal, that is when $h_1 = h_2$, the conditions are met since $A_{h_1, h_1} = B_{h_1, h_1} = 1$. Outside the diagonal they have to be derived from conditions on the design. Determining these conditions is an aim of this work. That is, given the Fourier model with frequencies in A we are concerned with finding a design, D orthogonal with respect to A . In condensed form our objects of interest are the model-design pairs (A, D) . We shall fully exploit this point in Chapter 5. Notice that given the model A the conditions (4.1) turn out to be the same for any A^+ defining A .

4.1.1 Examples of Fourier models

Although the theory holds in general our examples are from a particular class of models, the *complete models*. They are described in the following format

$$\text{ClassModel}(\text{Dimension}; \text{Order}_1, \dots, \text{Order}_{\text{Dimension}}; \text{Interactions})$$

where *Dimension* is the number of factors in the models ($x = (x_1, \dots, x_d)$), the factor x_i is present up to the frequency specified by *Order* (for all $i = 1, \dots, d$), and the maximum number of interactions allowed is *Interactions* and all of them must be included in the model. The following relationships must hold $\text{Dimension} \geq \text{Interactions} \geq 1$. The first equality holds for a complete interaction model and the second for an additive model. We list some subclasses of models we shall concentrate on.

The one-dimensional Fourier regression model $F(1; m; 1)$ is

$$E(Y(x)) = \mu(x) = \theta_0 + \sqrt{2} \sum_{r=1}^m \sin(2\pi r x) \theta_r + \sqrt{2} \sum_{r=1}^m \cos(2\pi r x) \phi_r \quad (4.2)$$

$x \in [0, 1)$. The frequency set A is then $\{-m, \dots, m\} \subset \mathbb{Z}$.

We call additive a model that does not include any interaction that is cross spectral terms and it includes all the marginal frequencies up to a certain order. A frequency set A^+ for additive models is formed by points on the coordinate axes:

$$A^+ = \left\{ \begin{array}{l} (h_1, 0, 0, \dots, 0) : h_1 = 1, \dots, m_1 \\ (0, h_2, 0, \dots, 0) : h_2 = 1, \dots, m_2 \\ \dots \\ (0, \dots, 0, 0, h_d) : h_d = 1, \dots, m_d \end{array} \right\}.$$

We use the notation $F(d; m_1, \dots, m_d; 1)$ to refer to this model. For example the two dimensional *additive model* $F(2; m_1, m_2; 1)$ is as follows

$$\begin{aligned} E(Y(x_1, x_2)) &= \mu(x_1, x_2) \\ &= \theta_0 + \sqrt{2} \sum_{r=1}^{m_1} \sin(2\pi r x_1) \theta_{1,r} + \sqrt{2} \sum_{r=1}^{m_1} \cos(2\pi r x_1) \phi_{1,r} \\ &\quad + \sqrt{2} \sum_{s=1}^{m_2} \sin(2\pi s x_2) \theta_{2,s} + \sqrt{2} \sum_{s=1}^{m_2} \cos(2\pi s x_2) \phi_{2,s}. \end{aligned} \quad (4.3)$$

For $m_1 = 4$ and $m_2 = 2$ the frequency set A is as in Figure 4.1. In general the additive model, $F(d; m_1, \dots, m_d; 1)$ is expressed by the formula

$$E(Y(x_1, \dots, x_d)) = \theta_0 + \sqrt{2} \sum_{k=1}^d \sum_{r_k=1}^{m_k} \sin(2\pi r_k x_k) \theta_{k,r_k} \quad (4.4)$$

$$+ \sqrt{2} \sum_{k=1}^d \sum_{r_k=1}^{m_k} \cos(2\pi r_k x_k) \phi_{k,r_k}. \quad (4.5)$$

The complete 2-factor interactions model, $F(d; m_1, \dots, m_d; 2)$ is

$$\begin{aligned} E(Y(x_1, \dots, x_d)) &= \theta_0 + \sqrt{2} \sum_{k=1}^d \sum_{r_k=1}^{m_k} \sin(2\pi r_k x_k) \theta_{k,r_k} + \sqrt{2} \sum_{k=1}^d \sum_{r_k=1}^{m_k} \cos(2\pi r_k x_k) \phi_{k,r_k} \\ &\quad + \sqrt{2} \sum_{k=1}^d \sum_{\ell=k+1}^d \sum_{r=1}^{m_k} \sum_{s=1}^{m_\ell} \sin(2\pi(r x_k + s x_\ell)) \theta_{k\ell,r,s}^+ \\ &\quad + \sqrt{2} \sum_{k=1}^d \sum_{\ell=k+1}^d \sum_{r=1}^{m_k} \sum_{s=1}^{m_\ell} \sin(2\pi(r x_k - s x_\ell)) \theta_{k\ell,r,s}^- \end{aligned}$$

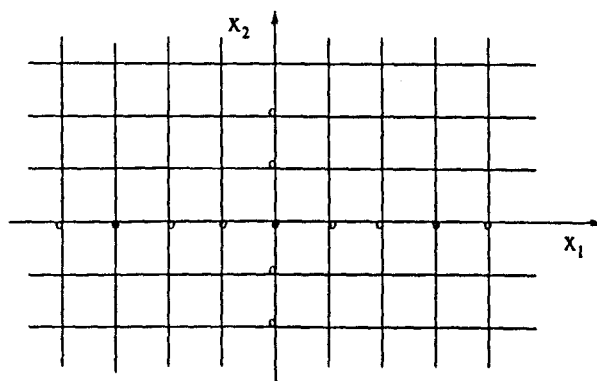


Figure 4.1: Frequency set for the additive model $m_1 = 4, m_2 = 2$.

$$\begin{aligned}
 & + \sqrt{2} \sum_{k=1}^d \sum_{\ell=k+1}^d \sum_{r=1}^{m_k} \sum_{s=1}^{m_\ell} \cos(2\pi(rx_k + sx_\ell)) \phi_{k\ell,rs}^+ \\
 & + \sqrt{2} \sum_{k=1}^d \sum_{\ell=k+1}^d \sum_{r=1}^{m_k} \sum_{s=1}^{m_\ell} \cos(2\pi(rx_k - sx_\ell)) \phi_{k\ell,rs}^- \quad (4.6)
 \end{aligned}$$

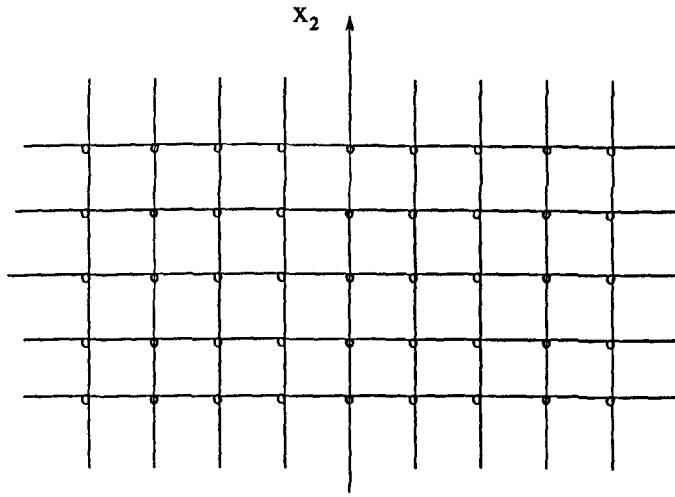
For example the model $F(d; 2, \dots, 2; 2)$ is a two-factor interaction model with marginal frequencies equal to 0, 1 and 2. A frequency set is

$$A^+ = \left\{ \begin{array}{cccc} (k, 0, \dots, 0) & (0, k, \dots, 0) & \dots & (0, \dots, k, 0) & (0, \dots, k) \\ (k, h, \dots, 0) & (0, k, h, \dots, 0) & \dots & (0, \dots, k, h) & \\ \dots & & & & \\ (k, 0, \dots, h) & (0, k, \dots, h) & \dots & & \end{array} \right\} : k, h = 1, 2$$

For example the two dimensional model $F(2; 4, 2; 2)$ is the model whose frequency set A is shown in Figure 4.2. Note that this is a complete interaction model or product model.

The above generalises to d -dimensions. If we introduce the sets $A_\ell = \{\alpha \in \{-1, 1\}^\ell; \alpha_1 = 1\}$ of all ℓ -dimensional multi-indices from $\{-1, 1\}$ with unit first entry, we can write the *product model* (complete interactions) $F(d; m_1, \dots, m_d; d)$ in the following form

$$\begin{aligned}
 & E(Y(x_1, \dots, x_d)) \\
 = & \theta_0 + \sqrt{2} \sum_{\ell=1}^d \sum_{k_1 < \dots < k_\ell} \sum_{r_{k_1}=1}^{m_{k_1}} \dots \sum_{r_{k_\ell}=1}^{m_{k_\ell}} \sum_{\alpha \in A_\ell} \sin(2\pi(\alpha_1 r_{k_1} x_{k_1} + \dots + \alpha_\ell r_{k_\ell} x_{k_\ell})) \\
 & \times \theta_{k_1 \dots k_\ell, r_{k_1} \dots r_{k_\ell}}^\alpha \\
 & + \sqrt{2} \sum_{\ell=1}^d \sum_{k_1 < \dots < k_\ell} \sum_{r_{k_1}=1}^{m_{k_1}} \dots \sum_{r_{k_\ell}=1}^{m_{k_\ell}} \sum_{\alpha \in A_\ell} \cos(2\pi(\alpha_1 r_{k_1} x_{k_1} + \dots + \alpha_\ell r_{k_\ell} x_{k_\ell})) \\
 & \times \phi_{k_1 \dots k_\ell, r_{k_1} \dots r_{k_\ell}}^\alpha \quad (4.7)
 \end{aligned}$$

Figure 4.2: Frequency set for $F(2; 4, 2; 2)$.

and the compact form for the complete M -factor interactions model, $F(d; m_1, \dots, m_d; M)$ is

$$\begin{aligned}
& E(Y(x_1, \dots, x_d)) \\
&= \theta_0 + \sqrt{2} \sum_{\ell=1}^M \sum_{k_1 < \dots < k_\ell} \sum_{r_{k_1}=1}^{m_{k_1}} \dots \sum_{r_{k_\ell}=1}^{m_{k_\ell}} \sum_{\alpha \in A_\ell} \sin(2\pi(\alpha_1 r_{k_1} x_{k_1} + \dots + \alpha_\ell r_{k_\ell} x_{k_\ell})) \\
&\quad \times \theta_{k_1 \dots k_\ell, r_{k_1} \dots r_{k_\ell}}^\alpha \\
&+ \sqrt{2} \sum_{\ell=1}^M \sum_{k_1 < \dots < k_\ell} \sum_{r_{k_1}=1}^{m_{k_1}} \dots \sum_{r_{k_\ell}=1}^{m_{k_\ell}} \sum_{\alpha \in A_\ell} \cos(2\pi(\alpha_1 r_{k_1} x_{k_1} + \dots + \alpha_\ell r_{k_\ell} x_{k_\ell})) \\
&\quad \times \phi_{k_1 \dots k_\ell, r_{k_1} \dots r_{k_\ell}}^\alpha. \tag{4.8}
\end{aligned}$$

Using the $F(2; m_1, m_2; 2)$ model we show that complete Fourier models are actually product of suitable marginals. Using standard formulae of trigonometry, which form an orthogonal transformation not affecting the D -, A -, E - and $IMSE$ -criteria, one regains the product of the marginals structure. Thus

$$\begin{aligned}
E(Y(x_1, x_2)) &= \theta_0 + \sqrt{2} \sum_{r=1}^{m_1} \sin(2\pi r x_1) \theta_{1,r} + \sqrt{2} \sum_{r=1}^{m_1} \cos(2\pi r x_1) \phi_{1,r} \\
&+ \sqrt{2} \sum_{s=1}^{m_2} \sin(2\pi s x_2) \theta_{2,s} + \sqrt{2} \sum_{s=1}^{m_2} \cos(2\pi s x_2) \phi_{2,s} \\
&+ 2 \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \sin(2\pi r x_1) \sin(2\pi s x_2) \theta_{r,s} \\
&+ 2 \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \sin(2\pi r x_1) \cos(2\pi s x_2) \lambda_{r,s} \\
&+ 2 \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \cos(2\pi r x_1) \sin(2\pi s x_2) \tau_{r,s}
\end{aligned}$$

$$+ 2 \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \cos(2\pi r x_1) \cos(2\pi s x_2) \phi_{rs} \tag{4.9}$$

is written as

$$\begin{aligned} E(Y(x_1, x_2)) = & \theta_0 + \sqrt{2} \sum_{r=1}^{m_1} \sin(2\pi r x_1) \theta_{1,r} + \sqrt{2} \sum_{r=1}^{m_1} \cos(2\pi r x_1) \phi_{1,r} \\ & + \sqrt{2} \sum_{s=1}^{m_2} \sin(2\pi s x_2) \theta_{2,s} + \sqrt{2} \sum_{s=1}^{m_2} \cos(2\pi s x_2) \phi_{2,s} \\ & + \sqrt{2} \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \sin(2\pi(r x_1 + s x_2)) \theta_{rs}^+ \\ & + \sqrt{2} \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \sin(2\pi(r x_1 - s x_2)) \theta_{rs}^- \\ & + \sqrt{2} \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \cos(2\pi(r x_1 + s x_2)) \phi_{rs}^+ \\ & + \sqrt{2} \sum_{r=1}^{m_1} \sum_{s=1}^{m_2} \cos(2\pi(r x_1 - s x_2)) \phi_{rs}^- \end{aligned} \tag{4.10}$$

Table 4.1 gives the number of parameters for complete models.

Model	Number of parameters
$F(1; m; 1)$	$2m + 1$
$F(2; m_1, m_2; 1)$	$2(m_1 + m_2) + 1$
$F(2; m_1, m_2; 2)$	$(2m_1 + 1)(2m_2 + 1)$
$F(d; m_1, \dots, m_d; 1)$	$1 + 2 \sum_{k=1}^d m_k$
$F(d; m_1, \dots, m_d; d)$	$\prod_{k=1}^d (2m_k + 1)$
$F(d; m_1, \dots, m_d; 2)$	$1 + 2 \sum_{k=1}^d m_k + 4 \sum_{j=1}^{d-1} m_j \sum_{k=j+1}^d m_k$
$F(d; m_1, \dots, m_d; M)$	$1 + 2 \sum_{k=1}^d m_k + 2^2 \sum_{j=1}^{d-1} m_j \sum_{k=j+1}^d m_k + \dots$ $\dots + 2^M \sum_{j_1=1}^{d-M+1} m_{j_1} \dots m_{j_{M-1}} \sum_{j_M=j_{M-1}+1}^d m_{j_M}$

Table 4.1: The dimension of some parameter vectors.

4.2 Optimum designs: background

From the above we require designs that are orthogonal with respect to certain Fourier models. From the well-established literature on experimental design we use the following properties.

Since the information matrix is diagonal, orthogonal designs are optimal with respect to any convex criterion based on the eigenvalues of the information matrix (a convex permutation invariant function of many variables is minimised when the variables are all equal, see Giovagnoli and Wynn, 1985 [33] and Giovagnoli, Pukelsheim and Wynn, 1987 [32]). In particular they are D -, A -, E -, IMS -optimal (or G -optimality). See Table 4.2 where $X^t X$ is the information matrix, max and min are taken over the design region and $E(\hat{Y}(x))$ is the predict value at x .

Optimality	Definition	Property
D	$\max X^t X$	Maximum of the power of the F -test for the parameter vector.
A	$\min \text{tr} X^t X$	Minimum of the sum of the variances of the least square estimators.
E	max min eigenvalue of $X^t X$	Estimation of all linear functions of the parameters.
G	$\min \int [E(Y(x)) - E(\hat{Y}(x))]^2 dx$	The best linear unbiased predictor.

Table 4.2: Optimality criteria.

All these criteria are invariant under orthogonal transformations of the design, and, by duality arguments, of the model, such as those that lead from Equation 4.9 to Equation 4.10. Moreover the D -optimality (and thus the G -optimality by the General Equivalence Theorem) is invariant under any linear transformation, that is it is independent of reparametrisations.

At times we are interested in estimating a subset of the parameter vector. For example $\beta = I_s \theta$ where I_s is a suitable rectangular matrix with 0 and 1 as entries that selects the required parameters. Instead of the inverse information matrix $(X^t X)^{-1}$ we have to consider $I_s (X^t X)^{-1} I_s^t$ and to talk of D_s -, A_s -, E_s -, G_s -optimality. For example we could be interested in estimating the parameters giving the main effect, or those representing interactions up to a certain order, say S .

For the one-dimensional model $F(1; m; 1)$ the uniform design supported on an equally spaced grid with at least $2m + 1$ points is D -optimum as we shall see (see also Kiefer, 1959, [39] and Pukelsheim, 1993 [54]). Moreover a minimal support design, that is a design with as many points as the number of parameters to be estimated, is the uniform design on any $2m + 1$ point grid.

Hoel (1965) [36] shows that *product designs* are D -optimal for product models. Thus, if ξ_1 is a D -optimum design measure for a linear model $E(Y) = \sum_{i=0}^{m_1} \theta_i f_i(x_1)$ on a design space X_1 and similarly ξ_2 is D -optimum for a model $E(Y) = \sum_{i=0}^{m_2} \phi_i g_i(x_2)$ on a space X_2 , then the product measure $\xi_1 \times \xi_2$ is D -optimum for the linear model whose terms are of the form $f_i(x_1)g_j(x_2)$ on the space $X_1 \times X_2$. The same is true for models in higher dimensions and with no interactions if $f_0 = 0$ and $g_0 = 0$ in general. For Fourier regression this last restriction is not necessary (see Schwabe, 1994 [65]). The same result for the other criteria has been proved for example by Rafajłowicz and Myszka (1992) [55] and Schwabe (1994) [66]. We consider uniform measures.

Products of D -optimal (and orthogonal) designs are still D -optimal for sums of models. But they present a major disadvantage in that they have too many points with respect to the number of parameters. For example consider the marginal models $F(1; m_1; 1)$ and $F(1; m_2; 1)$ and the uniform designs with $2m_1 + 1$ and $2m_2 + 1$ points uniformly distributed respectively. The size of the product design is $(2m_1 + 1)(2m_2 + 1)$ compared with the number of parameters in the sum model $2m_1 + 2m_2 + 1$ (see Kiefer, 1959, [39] and see also Pukelsheim, 1993, [54] for a recent textbook).

Again if the designs ξ_k are D -optimum (orthogonal) in the marginal models of the form (4.2) then the product type design $\xi_1 \times \dots \times \xi_d$ is D -optimum for all

the above multidimensional models (see for example Schwabe, 1993,1994b [64, 65]). The number of supporting points for $\xi_1 \times \dots \times \xi_d$ is at least $\prod_{k=1}^d (2m_k + 1)$ which is attained by a uniform design on a $(2m_1 + 1) \times \dots \times (2m_d + 1)$ equidistant grid in each component. In general the number of supporting points is much larger than the number of parameters. This design has minimal support only in the complete interaction model (4.7).

4.3 Lattice designs

We investigate lattice designs which are uniform designs supported on so-called integration lattices or lattice grids. These are used extensively in algebraic number theory and numerical integration. One can consider this work as an investigation of the role of lattices in functional estimation or approximation rather than integration. We refer the reader interested in the application of lattices to integration to Sloan and Joe (1994) [69] and Niederreiter (1992) [50]. We introduce lattice theory in a form convenient for our exposition.

Definition 25 *An infinite lattice L_∞ in \mathbb{R}^d is a discrete subset of \mathbb{R}^d closed under summation and subtraction. An infinite lattice is called integration infinite lattice if it includes \mathbb{Z}^d . A finite integration lattice is $L := L_\infty \cap [0, 1)^d$ where L is an infinite integration lattice. The order (number of elements) of a finite integration lattice is denoted by $N \in \mathbb{Z}_+^*$.*

We use the word lattice to refer to “finite integration lattice”. By definition an infinite lattice is an infinite Abelian group and in particular it contains all higher order frequencies (harmonics) of any member. Also a lattice is a group under the operation $x_1 \circ x_2 = \{x_1 + x_2\}$, where $\{x\}$ is the point in $[0, 1)^d$ whose coordinates are the fractional part of the coordinates of x . We work in particular with the so-called *good lattice points* or *one-generator lattices*.

Definition 26 *Let $g = (g_1, \dots, g_d) \in \mathbb{Z}^d$ and $N \in \mathbb{Z}_+^*$ then*

$$L_\infty := \left\{ \left\{ \frac{kg}{N} \right\} \oplus \mathbb{Z}^d : k \in \{0, \dots, N - 1\} \right\},$$

where \oplus denotes the direct sum, is a one-generator integration lattice. The set

$$L := L_\infty \cap [0, 1)^d$$

is called one-generator lattice (grid). The integer vector g is called the generator.

Assumption 1 *Without loss of generality we assume $g \in \mathbb{Z}_+^d$.*

Theorem 19 *Let g and N be as in Definition 26. The order of $L := L_\infty \cap [0, 1)^d$ is N if and only if the $\text{gcd}(N, g_1, \dots, g_d) = 1$.*

Proof. See Niederreiter, 1992 [50]. “ \Leftarrow ”: If $\text{gcd}(N, g_1, \dots, g_d) = 1$ then there exists at least one $j \in \{1, \dots, d\}$ such that $\text{gcd}(N, g_j) = 1$. Since the numbers $\frac{kg_j}{N} : k = 0, \dots, N - 1$ are all distinct and we are done.

" \implies ": By contradiction, let $\gcd(N, g_1, \dots, g_d) = l \neq 1$ then there exist k and l such that $0 < k, k + l < N$ and

$$\left\{ \frac{kg}{N} \right\} = \left\{ \frac{(k+l)g}{N} \right\}. \quad \blacksquare$$

Assumption 2 We assume $\gcd(N, g_1, \dots, g_d) = 1$.

Assumption 2 allows us to have $g_1 = 1$ without loss of generality. This can be achieved by a rearrangement of the generated design points. Note that Assumption 2 means that we consider designs without replications as in Part I.

Assumption 3 We assume $g_1 = 1$.

Definition 27 We refer to L in Definition 26 under the Assumption 2 as the one-generator lattice generated by g and with N points. We write $L_{g,N}$.

The one-generator lattice $L_{g,N}$ can be written as

$$\begin{aligned} L &= \left\{ \left\{ \frac{kg}{N} \right\} : k = 0, \dots, N-1 \right\} \\ &= \left\{ \left(\frac{kg_1 \bmod N}{N}, \dots, \frac{kg_d \bmod N}{N} \right) : k = 0, \dots, N-1 \right\}. \end{aligned}$$

The previous notation shows that a one-generator lattice is a cyclic group generated by $\frac{g}{N}$. According to the definition every point in a lattice is an equivalence class under the equivalence relation "fractional part". For the purpose of this work it is convenient to consider the representative of each class lying in the unitary hypercube. The vector g generates a finite number of line segments in the d -dimensional hypercube $[0, 1]^d$, that is the set $L = \{(tg_1 \bmod 1, \dots, tg_d \bmod 1); t \in \mathbb{R}\}$, on which the lattice is supported. Thus a one-generator lattice can be visualised as a set of equidistant points on a line wrapped around $[0, 1]^d$ interpreted as the d -dimensional torus.

Definition 28 A lattice design is a uniform design supported on a one-generator lattice grid.

We shall use the term lattice design and the symbol $L_{g,N}$ to indicate both the lattice design and its supporting points. This should not confuse since the context makes clear which we are considering.

The simplest example of a lattice is in one-dimension. The only one-generator lattice of order N is the following set

$$\left\{ \frac{k}{N} : k = 0, \dots, N-1 \right\}.$$

The generator is the vector (1). The following function in Splus returns the lattice generated by the generator vector g (its components are given in input) and with N (possibly not distinct) points.

```
OneGenLattDes_function(g,N)
{
```

```

design <- matrix(rep(g, N), ncol = length(g), byrow = T)
temp <- matrix(rep(1:N, length(g)), ncol = length(g))
if (!(GCD(g)==1)) return (((design * temp)%% N)/N,
                          "replications")
else return(((design * temp) %% N)/N)
}

```

where GCD is a macro that returns the greatest common divisors of the integer components of the vector in input. The previous version of the above Splus macro was 13 lines long. This short version is due to Tim Holliday.

An important tool is the so-called *dual lattice* in whose terms we shall express the orthogonality conditions for lattice designs on Fourier models.

Definition 29 *The dual lattice of a finite or infinite lattice L is defined as*

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

Note that the dual set L^\perp is itself an infinite, typically non integration, lattice and if $h \in L^\perp$ then $sh \in L^\perp$ for any integer s .

Lemma 1 *Let L be a finite or infinite lattice, then*

1. L^\perp is an infinite lattice.
2. $L^\perp \subset \mathbb{Z}^d$ if and only if $L \supset \mathbb{Z}^d$.
3. $L^\perp \supset \mathbb{Z}^d$ if and only if $L \subset \mathbb{Z}^d$.
4. If $L = L_{g,N}$ is a one-generator lattice, then

$$L_{g,N}^\perp = \{h \in \mathbb{Z}^d \text{ such that } h^t g \equiv 0 \pmod{N}\}.$$

Proof. The first three follow straight from the definition. To prove the last we proceed as follows. For a one-generator lattice $h \in L_{g,N}^\perp$ if (and only if) $h^t kg \equiv 0 \pmod{N}$ for all $k \in \mathbb{Z}$. Since the latter is true for all integers k , then it is equivalent to $h^t g \equiv 0 \pmod{N}$. ■

A geometric interpretation of the dual lattice is as follows. The dual of a lattice, L gives information about the hyperplanes of dimension $d - 1$ associated with L , specifically the planes of the form

$$h^t x = k \text{ such that } k \in \mathbb{Z} \text{ and } x \in L.$$

There are many different ways to draw a family of equally spaced parallel planes in which each point of the lattice is on one of the planes and each plane contains at least one point of the lattice. Every $h \in L^\perp$ is orthogonal to such a family and the distance between each plane is $1/||h||$ where $||h||$ is the Euclidean norm. In closely spaced planes points are sparsely distributed (see Sloan and Joe, 1994 [69]). The key to the theory is the next lemma.

Lemma 2 *Let L be a lattice with N points in the unit hypercube $[0, 1)^d$, then*

$$\frac{1}{N} \sum_{x \in L \cap [0,1)^d} e^{2\pi i h^t x} = \begin{cases} 1 & \text{if } h \in L^\perp \\ 0 & \text{otherwise.} \end{cases}$$

Proof. This lemma generalises to lattices the fact that the sum of a sinusoidal function over the N complex roots of the unity has value 0. The proof in the case of one-generator lattices is revealing. The easy part is proved as follows and is the same for any kind of lattices: if a frequency h belongs to the dual L^\perp then the function $e^{2\pi i x^t h}$ assumes values 1 for each $x \in L$, dividing by the number of lattice points in the unitary hypercube we are done. To prove the other part suppose $h \notin L^\perp$, then

$$\begin{aligned} \sum_{x \in L \cap [0,1]^d} e^{2\pi i x^t h} &= \sum_{j=0}^{N-1} e^{2\pi i \left\{ \frac{jg}{N} \right\}^t h} \\ &\text{(by definition of lattice)} \\ &= \sum_{j=0}^{N-1} e^{2\pi i \frac{jg}{N}^t h} \\ &\text{(because of the periodicity of the complex exponential)} \\ &= \sum_{j=0}^{N-1} e^{2\pi i j \frac{k}{N}} \\ &\text{(where } k = g^t h \text{ is different from zero since } h \notin L^\perp) \\ &= \sum_{l=0}^{N-1} e^{2\pi i \frac{l}{N}} \\ &\text{(which is known to be zero).} \end{aligned}$$

For the proof for multi-generator lattices we refer to Sloan and Joe (1994, Lemma 2.1) [69] and Niederreiter (1992, Lemma 5.21) [50] for a proof based on the group representations. ■

4.3.1 Multirank lattices

In this section we briefly sketch the use of lattices in integration theory as from Sloan and Joe (1994) [69] and Niederreiter (1992) [50] because the facts stated here clarify the assumptions and this is a good place to consider lattices from an algebraic point of view. In integration theory lattice methods are used as quadrature formulae for numerical evaluation of multiple integrals

$$\int_{[0,1]^d} f(x) dx$$

where f is one-periodic in each component that is

$$f(x) = f(x + c) \text{ for all } x \in \mathbb{R}^d \text{ and } c \in \mathbb{Z}^d \quad (4.11)$$

and it satisfies regularity conditions such as having a continuous periodic extension at the boundary. There are techniques to periodise a function f in order to make it satisfies (4.11). Sloan and Joe (1994) [69] give three of them. The integral of f is then approximated by the value of the quadrature formula over a lattice L

$$\frac{\sum_{x \in L} f(x)}{N}.$$

Lattices other than one-generator lattices are used in integration theory. The following theorem classifies $L \cap [0,1]^d$ for all L integration lattices. For the proof see Sloan and Joe Section 3.2.

Theorem 20 (Canonical form of a lattice) *Let L be a d -dimensional integration lattice with more than one point. There exist a unique positive integer r , $1 \leq r \leq d$ called rank and r integers $N_1, \dots, N_r > 1$, called invariants such that*

$$N_{k+1} \text{ divides } N_k \text{ for all } k = 1, \dots, r - 1$$

and there exist r vectors in \mathbb{Z}^d , which are linearly independent over the rationals, called generators, such that for all $k = 1, \dots, r$ the coordinates of g_k and N_k are relatively prime and

$$L \cap [0, 1)^d = \left\{ \left\{ h_1 \frac{g_1}{N_1} + \dots + h_r \frac{g_r}{N_r} \right\} : \text{for all } 0 \leq h_k \leq n_k - 1, \text{ for all } k = 1, \dots, r \right\}.$$

Moreover the order of L is $N = N_1 \dots N_r$.

Note that the g_i 's are not uniquely defined. With the notation in the above theorem to a lattice L of rank r we can associate a full rank matrix M of dimension $r \times d$ whose i -th row is the vector $\frac{g_i}{N_i}$ for all $i = 1, \dots, r$. After possibly rearranging the column of M , that is the factors, we can write

$$M = (B, C)$$

where B is invertible of dimension $r \times r$. This matrix can be expanded to a full rank matrix, M_L of dimension $d \times d$ adding $d - r$ rows of integers. The invariant associated with a new generator is such that no new point is added to the lattice, only $(0, \dots, 0)$ which is replicated $d - r$ times. For example a generator matrix corresponding to the one-generator lattice $L_{(g_1, \dots, g_d), N}$ is

$$\begin{pmatrix} \frac{g_1}{N} & \dots & \frac{g_d}{N} \\ 0 & & I \end{pmatrix}$$

where I is the $(d - 1) \times (d - 1)$ identity matrix. In general we can choose M as follows

$$M = \begin{pmatrix} B & C \\ 0 & I \end{pmatrix}$$

where I is the identity matrix of dimension $d - r$. Thus the lattice point $\left\{ h_1 \frac{g_1}{N_1} + \dots + h_r \frac{g_r}{N_r} \right\}$ is given by the following scalar product

$$\{(h_1, \dots, h_r, h_{r+1}, \dots, h_d) M_L\}$$

where h_k is any integer for all $k = r + 1, \dots, d$. Recall that the curly brackets give the vector whose components are the rational part of the components of the vector inside the brackets.

Theorem 21 *Let M_L be a generator matrix of L then $(M_L^{-1})^t$ is the generator matrix of L^\perp .*

Proof. We have that

$$M_L^{-1} = \begin{pmatrix} B^{-1} & -B^{-1}C \\ 0 & I \end{pmatrix}.$$

Then we have that $p \in L$ if and only if there exist suitable integers such that $p = \{(h_1, \dots, h_d)M_L\}$ and $q \in L^\perp$ if and only if $q = (k_1, \dots, k_d)(M_L^{-1})^t$ for any integer vector (k_1, \dots, k_d) . The scalar product of p and q gives $(h_1, \dots, h_d)(k_1, \dots, k_d)^t \in \mathbb{Z}$ and we are done. ■

For example consider the two-dimensional lattice generated by $(\frac{1}{3}, \frac{2}{3})$ and $(\frac{2}{9}, \frac{5}{9})$. It is a rank 2 lattice and a generator matrix is

$$M_L = \begin{pmatrix} \frac{1}{3} & \frac{2}{3} \\ \frac{2}{9} & \frac{5}{9} \end{pmatrix}.$$

Its dual is generated by $f_1 = (15, -6)$ and $f_2 = (-18, 9)$. The lattice points are

$$L = \{\{kg_1 + hg_2\} : k, h \in \mathbb{Z}\} = \left\{ \left\{ \frac{3k(1, 2) + h(2, 5)}{9} \right\} : k, h \in \mathbb{Z} \right\}.$$

$9x_1$	$9x_2$	$9x_1$	$9x_2$	$9x_1$	$9x_2$
0	0	3	6	6	3
2	5	5	2	8	8
4	1	7	7	1	4
6	6	0	3	3	0
8	2	2	8	5	5
1	7	4	4	7	1
3	3	6	0	0	6
5	8	8	5	2	2
7	4	1	1	4	7

The following theorems (for whose proof we refer to Sloan and Joe, 1994 [69]) give a decomposition of a lattice L as the direct sum of lattices whose orders correspond to the prime factorisation of the order of L .

Theorem 22 *Let L be an integration lattice and N the cardinality of $L \cap [0, 1)^d$. Let $N = N_1 N_2$ be a non trivial factorisation of N such that N_1 and N_2 are relatively prime. There exist L_1 and L_2 integration lattices such that*

$$\#L_1 \cap [0, 1)^d = N_1 \text{ and } \#L_2 \cap [0, 1)^d = N_2$$

and L is direct sum of L_1 and L_2 and it is defined as follows

$$L = L_1 \oplus L_2 := \{x_i + y_j : x_i \in L_1 \text{ for all } 1 \leq i \leq N_1 \text{ and } y_j \in L_2 \text{ for all } 1 \leq j \leq N_2\}.$$

In particular

$$L \cap [0, 1)^d := \{\{x_i + y_j\} : x_i \in L_1 \text{ for all } 1 \leq i \leq N_1 \text{ and } y_j \in L_2 \text{ for all } 1 \leq j \leq N_2\}.$$

Note that with the notation of the previous theorem $N = N_1 N_2$. To deal with the case when N does not factorise as mutually prime numbers we consider without loss of generality the case $N = p^\gamma$ for some prime p and positive integer γ .

Theorem 23 *Let L be an integration lattice with $N = p^\gamma$ elements. There exist $v \in \mathbb{Z}_+$ and $n_1, \dots, n_v \in \mathbb{Z}_+$ such that $\sum_{k=1}^v n_k = \gamma$ and there exist L_1, \dots, L_v cyclic subgroups of L such that*

$$\#L_k = n_k \text{ for all } k = 1, \dots, v$$

and

$$L \cap [0, 1)^d = L_1 \oplus \dots \oplus L_v.$$

4.3.2 The error for quadrature formulae based on lattices

In most applications the function to be integrated is regular enough to let us assume it admits a Fourier series, thus

$$f(x) = \sum_{h \in \mathbf{Z}^d} \hat{f}(h) e^{2\pi i x^t h}$$

where

$$\hat{f}(h) = \int_{[0,1]^d} f(x) e^{-2\pi i x^t h} dx$$

and in particular for $h = (0, \dots, 0)$ we obtain the integral of f . A lattice quadrature formula assumes the form

$$Q(f) = \sum_{h \in \mathbf{Z}^d} \hat{f}(h) \frac{1}{N} \sum_{x \in L} e^{2\pi i x^t h}.$$

Thus the error to be minimised which is defined as $Q(f) - \int_{[0,1]^d} f(x) dx$ becomes

$$\sum_{h \in \mathbf{Z}^d \setminus \{0\}} \hat{f}(h) \frac{1}{N} \sum_{x \in L} e^{2\pi i x^t h}.$$

By Lemma 2 it simplifies to

$$\sum_{h \in L^\perp \setminus \{0\}} \hat{f}(h).$$

Thus every quadrature formula based on lattice points integrates exactly the majority of Fourier terms. It does not integrate exactly only for the frequencies h belonging to the dual lattice. In Section 5.4 we shall exploit Lemma 2 in a similar fashion.

Summary

In Part II of the thesis we are interested in Model/Design pairs where the model is a Fourier model and the design is a lattice design orthogonal for the model.

In this chapter we introduce complete Fourier linear models as an alternative to polynomial linear models in multivariate regression from a design of experiments point of view. A model is represented by a finite set of integer vectors referred to as a frequency set. These models are periodic in $[0, 1]^d$ and the completeness of the frequency set allows us to exploit the complex representation. In particular we concentrate on the orthogonality structure of the complex information matrix Z^*Z .

Orthogonal designs for Fourier models are sought within the class of designs supported on lattice grids (well known from number theory and group theory). They are defined by three elements: the rank, the set of generators and the sample size. The definitions and properties used in the subsequent chapters are stated and discussed.

Chapter 5

Orthogonality of lattice designs for Fourier models

The cyclic structure of one-generator lattice designs and Lemma 2 in Chapter 4 suggest some affinity with trigonometric functions. Indeed due to the periodic structure of one-generator lattice designs we are able to infer their orthogonality for Fourier models.

We first consider the one-dimensional case. We show a construction of multi-dimensional orthogonal designs based on considerations on the projections (marginal designs) that leads to lattice designs. We then state the main theorems and in particular give necessary and sufficient conditions for a one-generator lattice to be orthogonal with respect to a certain Fourier model. These same theorems will then be translated into algebraic terminology which gives a different perspective.

Let m be a non-negative integer. Define the symbols $\mathcal{N}_m := \{r : r = -m, \dots, -1, 0, 1, \dots, m\}$ and $\mathcal{N}_m^* := \{r : r = -m, \dots, -1, 1, \dots, m\}$. We use \mathcal{G}_m for the additive group over $\{0, \dots, m-1\}$.

For the one-dimensional Fourier model, the following theorem was stated in for example Kiefer (1959) [39] and Pukelsheim (1993) [54].

Theorem 24 *For the model $F(1; m; 1)$ the lattice design generated by $g \in \mathbb{Z}$ and with N supporting points ($N \geq 2m + 1$) is D -optimum if and only if $2m + 1$ is the cardinality of $g\mathcal{N}_m$ considered as a subset of the cyclic group \mathcal{G}_N .*

Proof. Indeed $F(1; m; 1)$ at the design point $\frac{k}{2m+1}$ is

$$\sum_{h=-m}^m \delta_h e^{2\pi i h \frac{k}{2m+1}} \text{ for all } k = 0, \dots, 2m.$$

The (k, l) -th element of the complex information matrix is

$$(Z^*Z)(k, l) = \sum_{h=-m}^m \delta_h e^{2\pi i h \frac{-k+l}{2m+1}} = \begin{cases} 2m + 1 & \text{if } k = l \\ 0 & \text{otherwise.} \end{cases} \quad \blacksquare$$

The proof of analogous theorems for the multidimensional case requires the following theorem in which we consider the situation when only a subset of parameters has to be estimated.

Theorem 25 For the incomplete one-dimensional Fourier model

$$E(Y(x)) = \theta_0 + \sqrt{2} \sum_{j=1}^q \sin(2\pi r_j x) \theta_j + \sqrt{2} \sum_{j=1}^q \cos(2\pi r_j x) \phi_j \quad (5.1)$$

where the r_j are distinct positive integers, the N -point lattice design generated by g is D -optimum for the subsystem $(\theta_0, \theta_1, \phi_1, \dots, \theta_p, \phi_p)$ of parameters, $p \leq q$, if and only if, within the cyclic group $\mathcal{G}_N = (\{0, 1, \dots, N-1\}, +)$, (i) the cardinality of the set $\{0\} \cup g\mathcal{N}'$ is $2p+1$, where $\mathcal{N}' = \{\pm r_j; j = 1, \dots, p\}$, and (ii) $r_j \notin \{0\} \cup g\mathcal{N}'$ for $j = p+1, \dots, q$.

Proof. As in Lemma 2 we have 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, $r \neq -s \pmod{N}$. 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 $(\theta_0, \theta_1, \phi_1, \dots, \theta_p, \phi_p)$ of parameters is involved. Thus, by a simple refinement of the argument the design is also D -optimum for the subsystem in the full model. The converse can be checked by noting that for either $r = s \pmod{N}$ or $r = -s \pmod{N}$ the corresponding rows of the information matrix are linearly dependent and thus the parameters cannot be identified. ■

5.1 Motivation

A key observation is that a model with terms in higher dimensions can be “tricked” into a model in one-dimension by exploiting the structure of lattice designs. We explain this with a two dimensional example. Consider the model $F(2; 1, 1; 2)$ which has 9 parameters and the lattice with generator $(1, 3)$ and $N = 9$ supporting points. The second variable of the lattice points assumes only the values $0, \frac{1}{3}, \frac{2}{3}$ while the first one covers all the values $\frac{k}{9}$ for all $k = 0, \dots, 9$. The four ways in which the variables are “combined” are

$$x_1, \quad x_2, \quad x_1 + x_2, \quad x_1 - x_2.$$

Associating x_1 to $g_1 = 1$, x_2 to $g_2 = 3$ and multiplying by $k \in \{0, \dots, 8\}$ we generate the following column vectors of the design matrix multiplied by 9

$x_1 \pmod{9}$	$x_2 \pmod{9}$	$(x_1 + x_2) \pmod{9}$	$(x_1 - x_2) \pmod{9}$
0	0	0	0
1	3	4	7
2	6	8	5
3	0	3	3
4	3	7	1
5	6	2	8
6	0	6	6
7	3	1	4
8	6	5	2

Identical columns would be produced by a *one-dimensional model* with only the terms $r = 1, r = 3, r = 4, r = 7$ and equally spaced observations, that is the model $F(2; 1, 1; 2)$ is tricked into the one-dimensional non-complete Fourier model with regression function

$$\left(1, \cos(2\pi x), \cos(2\pi 3x), \cos(2\pi 4x), \cos(2\pi 7x), \right. \\ \left. \sin(2\pi x), \sin(2\pi 3x), \sin(2\pi 4x), \sin(2\pi 7x) \right)^t.$$

By Theorem 25 for this last model the uniform design with 9 equispaced supporting points is orthogonal. Since the information matrix for $F(2; 1, 1; 2)$ evaluated in the lattice design $L_{(1,3),9}$ is equal to the information matrix for the non-complete model evaluated in the 9 point uniform design, we conclude that the given lattice design is orthogonal for $F(2; 1, 1; 2)$.

Notice that according to Theorem 25 in considering the sequence $(1, 3, 4, 7)$ it is critical that in the full sequence $(1, 3, 4, 7, 9-7=2, 9-4=5, 9-3=6, 9-1=8)$ there are no repetitions. We require that in the cyclic group \mathcal{G}_9 the elements of the sequence $(-6, -5, -4, -1, 1, 4, 5, 6)$ are unique values.

The same design $L_{(1,3),9}$ is also orthogonal for the 2-dimensional Fourier models with frequency set $A = \{(1, 0), (0, 1), (2, 0), (1, 1)\}$, that is

$$E(Y) = \theta_0 + \theta_{1,1} \sin(2\pi r x_1) + \phi_{1,1} \cos(2\pi r x_1) + \theta_{1,2} \sin(4\pi r x_1) + \phi_{1,2} \cos(4\pi r x_1) \\ + \theta_{2,1} \sin(2\pi r x_2) + \phi_{2,1} \cos(2\pi r x_2) \\ + \theta_{2,2} \sin(2\pi r(x_1 + x_2)) + \phi_{2,2} \cos(1\pi r(x_1 + x_2)).$$

In particular $\pm g_1, \pm g_2, \pm 2g_1, \pm(g_1 + g_2)$ correspond to $\pm 1, \pm 3, \pm 2, \pm 4$ respectively and these are distinct (mod 9). Both models are saturated with respect to the design $L_{(1,3),9}$ that is the number of design points equals the number of parameters.

5.2 Another example: complete interaction models

Let us consider $F(2; m_1, m_2; 2)$. A particular orthogonal design is given by $\xi_1^* \times \xi_2^*$ which is uniform on the $(2m_1+1) \times (2m_2+1)$ grid $\{(\frac{i}{2m_1+1}, \frac{j}{2m_2+1}), i = 0, \dots, 2m_1, j = 0, \dots, 2m_2\}$.

We fix ξ_2^* and look for different D -optimum designs in the following way. For any supporting design point x_2 of ξ_2^* we can take any D -optimum marginal design $\xi_{1|x_2}^*$ without changing the information matrix. Now we can consider $\xi_{1|x_2}^*$ as a conditional design (conditioned on x_2). This concept is further explained in Cook and Thibodeau (1980) [23] and, more generally, Kurotschka (1984) [43]. Then $\xi_{1|x_2}^*$ is a conditional probability measure and $\xi_{1|x_2}^* \times \xi_2^*$ defines a new design in $[0, 1]^d$ which is itself D -optimum.

In particular, let $\xi_{1|x_2}^*$ given $x_2 = \frac{j}{2m_2+1}$ be uniform on

$$\left\{ \frac{i}{2m_1+1} + \frac{j}{(2m_1+1)(2m_2+1)}; i = 0, \dots, 2m_1 \right\}$$

then $\xi^* = \xi_{1|x_2}^* \times \xi_2^*$ is uniform on

$$\left\{ \left(\frac{1}{2m_1+1} \left(i + \frac{j}{2m_2+1} \right), \frac{j}{2m_2+1} \right); i = 0, \dots, 2m_1, j = 0, \dots, 2m_2 \right\}.$$

After a rearrangement of the design points we see that ξ^* is uniform on

$$\left\{ \left(\frac{k}{N}, \frac{k(2m_1 + 1) \bmod N}{N} \right); k = 0, \dots, N - 1 \right\}$$

where $N = (2m_1 + 1)(2m_2 + 1)$ is the number of supporting points. This concept can be generalised to higher dimensions.

In summary the grid $(2m_1 + 1) \times (2m_2 + 1)$ is generated by the one generator lattice $(1, 2m_1 + 1)$ with $N = (2m_1 + 1)(2m_2 + 1)$ points.

5.3 Complete models

The general result of this section is Theorem 26 whose proof follows directly from the theory of Section 5.4. The other theorems are specialisations of it for particular classes of Fourier models, which will be useful in the examples of Chapter 6.

Theorem 26 *In the M -factor interaction model $F(d; m_1, \dots, m_d; M)$ the N -point lattice design generated by (g_1, \dots, g_d) is orthogonal 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*

$$\begin{array}{l} 0, \\ \tau_k g_k, \quad \tau_k \in \mathcal{N}^*_{k_1}, \quad k = 1, \dots, d \\ \tau_k g_k + \tau_\ell g_\ell, \quad \tau_k \in \mathcal{N}^*_{k_1} \text{ and } \tau_\ell \in \mathcal{N}^*_{\ell_1}, \quad 1 \leq k < \ell \leq d \\ \vdots \\ \tau_{k_1} g_{k_1} + \dots + \tau_{k_m} g_{k_m}, \quad \tau_{k_1} \in \mathcal{N}^*_{k_1}, \dots, \tau_{k_m} \in \mathcal{N}^*_{k_m}, \quad 1 \leq k_1 < \dots < k_m \leq d \\ \vdots \\ \tau_{k_1} g_{k_1} + \dots + \tau_{k_M} g_{k_M}, \quad \tau_{k_1} \in \mathcal{N}^*_{k_1}, \dots, \tau_{k_M} \in \mathcal{N}^*_{k_M}, \quad 1 \leq k_1 < \dots < k_M \leq d, \end{array}$$

where $\mathcal{N}^*_{k_1} = \{-m_{k_1}, \dots, -1, 1, \dots, m_{k_1}\}$, are distinct in the cyclic group \mathcal{G}_N and additionally (for $S < M$) they are different in \mathcal{G}_N from the members in the last $M - S$ rows.

Theorem 27 *The lattice design generated by (g_1, g_2) and with N supporting points is orthogonal for the model $F(2; m_1, m_2; 2)$ if and only if all sums*

$$\tau g_1 + s g_2; \quad \tau \in \mathcal{N}_{m_1}, s \in \mathcal{N}_{m_2}$$

are distinct in the cyclic group \mathcal{G}_N .

Theorem 28 *For the model $F(d; m_1, \dots, m_d; d)$ the lattice design generated by (g_1, \dots, g_d) and with N supporting points is orthogonal if and only if all the sums*

$$\tau_1 g_1 + \dots + \tau_d g_d; \quad \tau_1 \in \mathcal{N}_{m_1}, \dots, \tau_d \in \mathcal{N}_{m_d}$$

are distinct in the cyclic group \mathcal{G}_N .

Theorem 29 For the model $F(d; m_1, \dots, m_d; M)$ the lattice design generated by (g_1, \dots, g_d) and with N supporting points is orthogonal if and only if the members of the following array are distinct in the cyclic group \mathcal{G}_N

$$\begin{array}{l}
0, \\
\tau_k g_k, \quad \tau_k \in \mathcal{N}_{m_k}^*, \quad k = 1, \dots, d \\
\tau_k g_k + \tau_\ell g_\ell, \quad \tau_k \in \mathcal{N}_{m_k}^*, \tau_\ell \in \mathcal{N}_{m_\ell}^*, \quad 1 \leq k < \ell \leq d \\
\vdots \\
\tau_{k_1} g_{k_1} + \dots + \tau_{k_m} g_{k_m}, \quad \tau_{k_1} \in \mathcal{N}_{m_{k_1}}^*, \dots, \tau_{k_m} \in \mathcal{N}_{m_{k_m}}^*, \quad 1 \leq k_1 < \dots < k_m \leq d \\
\vdots \\
\tau_{k_1} g_{k_1} + \dots + \tau_{k_M} g_{k_M}, \quad \tau_{k_1} \in \mathcal{N}_{m_{k_1}}^*, \dots, \tau_{k_M} \in \mathcal{N}_{m_{k_M}}^*, \quad 1 \leq k_1 < \dots < k_M \leq d.
\end{array}$$

In particular, for additive models only the members of the first two rows of the array have to be different. For a two-factor interaction model only the elements in the first three rows of the array have to be different, and for complete interaction models we recover the conditions in Theorems 27 and 28. Next we investigate the situation in which only the main effects are involved.

Theorem 30 For the parameters associated with the main effects of the model $F(d; m_1, \dots, m_d; M)$ the lattice design generated by (g_1, \dots, g_d) and with N supporting points is orthogonal if and only if the members in the first two rows

$$\begin{array}{l}
0, \\
\tau_k g_k, \quad \tau_k = -m_k, \dots, -1, 1, \dots, m_k, \quad k = 1, \dots, d
\end{array}$$

of the array

$$\begin{array}{l}
0, \\
\tau_k g_k, \quad \tau_k = -m_k, \dots, -1, 1, \dots, m_k, \quad k = 1, \dots, d \\
\tau_k g_k + \tau_\ell g_\ell, \quad \tau_k = -m_k, \dots, -1, 1, \dots, m_k, \\
\quad \tau_\ell = -m_\ell, \dots, -1, 1, \dots, m_\ell, \quad 1 \leq k < \ell \leq d \\
\vdots \\
\tau_{k_1} g_{k_1} + \dots + \tau_{k_m} g_{k_m}, \quad \tau_{k_1} \in \mathcal{N}_{m_{k_1}}^*, \dots, \tau_{k_m} \in \mathcal{N}_{m_{k_m}}^*, \quad 1 \leq k_1 < \dots < k_m \leq d \\
\vdots \\
\tau_{k_1} g_{k_1} + \dots + \tau_{k_M} g_{k_M}, \quad \tau_{k_1} \in \mathcal{N}_{m_{k_1}}^*, \dots, \tau_{k_M} \in \mathcal{N}_{m_{k_M}}^*, \quad 1 \leq k_1 < \dots < k_M \leq d
\end{array}$$

are distinct in the cyclic group \mathcal{G}_N and, additionally, the members in the others rows are all different to the members in the first two rows (in \mathcal{G}_N).

5.4 Mutually orthogonal frequencies

Lemma 2 in Section 4.3 gives conditions for complete orthogonality which we present in the following theorem. The proof follows immediately from it. Note that the complete orthogonality is more easily expressed via the complex design matrix Z .

Theorem 31 Consider the Fourier model defined by the set of frequencies A . Let A^+ be one of the sets giving A . For a one-generator lattice, L with generator g and N points, the complex design matrix, Z satisfies $Z^*Z = NI$, complete orthogonality, if and only if the following three conditions are satisfied

- (i) $h_1 \notin L^\perp$
- (ii) $(h_1 - h_2) \notin L^\perp$ with $h_1 \neq h_2$
- (iii) $(h_1 + h_2) \notin L^\perp$

for all h_1, h_2 frequencies in the Fourier regression model A ; equivalently if and only if

- (i*) $(h_1 - h_2) \notin L^\perp$ for all $h_1, h_2 \in A$ with $h_1 \neq h_2$.

Note that (iii) requires in particular $2h_1 \notin L^\perp$, which is in turn implied by (i) and (ii) if N is odd.

Assumption 4 To avoid additional technicalities we assume N odd, unless otherwise stated.

Thus (iii) simplifies to $h_1 + h_2 \notin L^\perp$ for $h_1 \neq h_2$. It is convenient to express the orthogonality as a pairwise property between different frequencies h_1, h_2 .

Definition 30 A pair of frequencies (h_1, h_2) is called mutually orthogonal (with respect to the lattice L) if $h_1, h_2 \notin L^\perp$ and $\pm h_1 \pm h_2 \notin L^\perp$.

Note that the above definition implies $h_1 \neq h_2$ for orthogonal h_1 and h_2 . The following theorem summarises all the above.

Theorem 32 If every pair $h_1, h_2 \in A^+$ is mutually orthogonal with respect to L^\perp then L is completely orthogonal for the model $A = A^+ \cup \{-A^+\} \cup \{0\}$.

5.5 Double cosets

In this section we present a necessary and sufficient condition for a pair $h_1, h_2 \in A^+$ to be mutually orthogonal which is similar to the condition of not being aliased in factorial experimental design. It is of historic interest that the term alias occurs both in the time series/signal processing literature and in the experimental design literature. That this analogy applies in the one-dimensional case is well-known. We believe that the present extension to lattice designs is new. For readers acquainted with the classical development of the alias table in experimental design the following development in terms of cosets will be familiar. Note however how the Fourier model expressed as $A^+ \cup \{-A^+\}$ gives a double coset interpretation of aliasing. We need to recall some elementary group theory.

Let $(G, +)$ be an Abelian group, U a subgroup of G and a an element of G . The set $K_a = K - a := \{-a + u : u \in U\}$ is called the a -coset of G with respect to U . More precisely the equivalence relation on G defined by $a \sim b$ if $-a + b \in U$ generates the quotient G/U whose elements are the cosets of G with respect to U . Thus the cosets form a partition of G . It turns out that the orthogonality conditions in Theorem 31 are related to pairs of cosets $K_a \cup K_{-a}$. We denote by L_h^\perp the h -coset of L^\perp in \mathbb{Z}^d .

Theorem 33 *The frequencies h_1 and h_2 are mutually orthogonal if and only if there exist $h \notin L^\perp$ and $h' \notin L^\perp$ such that $h_1 \in L_h^\perp \cup L_{-h}^\perp$ and $h_2 \in L_{h'}^\perp \cup L_{-h'}^\perp$, and the two double cosets are disjoint.*

We note that the notation L_h^\perp means $(L^\perp)_h$ and is not to be confused with $(L_h)^\perp$ since (L_h) is not a lattice/group to which one applies the dual operator $^\perp$.

Proof. Let h_1 and h_2 be mutually orthogonal. By contradiction assume that h_1 and h_2 are in the same double coset $L_h^\perp \cup L_{-h}^\perp$. Without loss of generality $h_1 \in L_h^\perp$ and, hence, $h_1 - h \in L^\perp$. We also have either $h_2 - h \in L^\perp$ or $h_2 + h \in L^\perp$. As L^\perp is a group it follows $h_1 - h_2 \in L^\perp$ or $h_1 + h_2 \in L^\perp$ which contradicts the assumption. This proves the direct part.

Conversely, if h_1 and h_2 are not mutually orthogonal, then either $h_1 - h_2 \in L^\perp$ or $h_1 + h_2 \in L^\perp$. Hence, $h_1 \in L_{h_2}^\perp \cup L_{-h_2}^\perp$ which shows that h_1 and h_2 are in the same double coset. ■

Next we consider cosets for the dual lattice of a one-generator lattice design L with N points, N odd and $g_1 = 1$. Thus the lattice is

$$L = \left\{ \frac{k(1, g_2, \dots, g_d) \pmod{N}}{N} : k = 0, \dots, N-1 \right\}$$

and its dual is

$$L^\perp = \left\{ (a_1, \dots, a_d) \in \mathbb{Z}^d : (a_1, \dots, a_d)(1, \dots, g_d)^t \equiv 0 \pmod{N} \right\}.$$

The (h_1, \dots, h_d) -coset is

$$L_{(h_1, \dots, h_d)}^\perp = \left\{ (a_1 - h_1, \dots, a_d - h_d) \in \mathbb{Z}^d : (a_1, \dots, a_d) \in L^\perp \right\}.$$

It turns out that there are N cosets forming a partition of \mathbb{Z}^d : the proof follows immediately from Theorem 34 below. We can enumerate them as

$$L_{(0, \dots, 0)}^\perp, L_{(1, \dots, 0)}^\perp, \dots, L_{(N-1, \dots, 0)}^\perp$$

and for notational convenience we write $L_k^\perp = L_{(k, \dots, 0)}^\perp$ for $k = 0, \dots, N-1$ where L_0^\perp is L^\perp itself. The following theorem characterises the double cosets for a one-generator lattice.

Theorem 34 *For the lattice L with N points and generated by $g = (1, g_2, \dots, g_d)$, $L_{(h_1, \dots, h_d)}^\perp = L_k^\perp$ if and only if $h_1 + g_2 h_2 + \dots + g_d h_d \equiv k \pmod{N}$.*

Proof. It holds that $h = (h_1, \dots, h_d) \in L_h^\perp$ if and only if

$$\begin{aligned} h &= (a_1 - k, a_2, \dots, a_d) \\ &= (b_1 - h_1, \dots, b_d - h_d) \end{aligned}$$

for some $(a_1, \dots, a_d), (b_1, \dots, b_d) \in L^\perp$. Equivalently if and only if

$$(a_1, a_2, \dots, a_d) = (b_1 - h_1 + k, b_2 - h_2, \dots, b_d - h_d) \in L^\perp.$$

This condition expands and is equivalent to

$$(b_1 - h_1 + k) + g_2(b_2 - h_2) + \dots + g_d(b_d - h_d) \equiv 0 \pmod{N}.$$

Since $(b_1, \dots, b_d) \in L^\perp$ the previous equation holds if and only if

$$-(h_1 + h_2g_2 + \dots + g_d h_d) + k \equiv 0 \pmod{N}.$$

That is $(h_1 + h_2g_2 + \dots + g_d h_d) \equiv k \pmod{N}$. ■

We determine the solutions in an empirical manner.

Since N is odd there are $\frac{N-1}{2}$ double cosets plus L^\perp itself, specifically

$$L^\perp, L_1^\perp \cup L_{N-1}^\perp, \dots, L_k^\perp \cup L_{N-k}^\perp, \dots, L_{\frac{N-1}{2}}^\perp \cup L_{\frac{N+1}{2}}^\perp \quad (k = 2, \dots, \frac{N-3}{2}).$$

This fact is of course clear from the underlying group theory.

Theorem 33 can be reformulated as h_1 and h_2 are mutually orthogonal if and only if $h_1^t g \neq 0$ and $h_2^t g \neq 0$ and

$$h_1^t g = h_{1_1} + g_2 h_{1_2} + \dots + g_d h_{1_d} \neq \pm (h_{2_1} + g_2 h_{2_2} + \dots + g_d h_{2_d}) = h_2^t g \pmod{N}.$$

Note that any frequency such that $h_1^t g = 0$ allows us to identify the constant term. Lemma 2 in Section 4.3 implies that if the model contains any two pairs of frequencies which are *not* mutually orthogonal with respect to the lattice design then Z (and X) becomes singular, that is the model as a whole is not identifiable. Thus to be fully identifiable by a lattice design with N points and generated by $(1, g_2, \dots, g_d)$ models can have at most $\frac{N-1}{2}$ terms and for every chosen $k = 0, \dots, \frac{N-1}{2}$ at most one model-frequency satisfies the equation

$$h_{1k} + g_2 h_{2k} + \dots + g_d h_{dk} \equiv k \pmod{N}.$$

This is not surprising since with a N point design we know that we can estimate a linear model with at most N parameters, that is an estimable Fourier model can have at most $\frac{N-1}{2}$ distinct frequencies (compare with Section 3.2).

As an example consider the two dimensional lattice generated by $(1, 5)$ and with 13 points. The lattice design supported on $L_{(1,5),13}$ is completely orthogonal for the model defined by $A = \{(1,0), (0,1), (1,1), (1,-1)\}$ because its frequencies generate respectively

$$\begin{aligned} L_{(1,0)}^\perp \cup L_{(12,0)}^\perp & \quad (1 + 5 \cdot 0 \equiv 1 \pmod{13}) \\ L_{(5,0)}^\perp \cup L_{(8,0)}^\perp & \quad (0 + 5 \equiv 5 \pmod{13}) \\ L_{(6,0)}^\perp \cup L_{(7,0)}^\perp & \quad (1 + 5 \equiv 6 \pmod{13}) \\ L_{(4,0)}^\perp \cup L_{(9,0)}^\perp & \quad (1 - 5 \equiv -4 = 9 \pmod{13}). \end{aligned}$$

The same design also identifies the saturated model

$$A = \{(1,0), (2,0), (0,1), (1,1), (1,-1), (2,-1)\}.$$

As another example the lattice design generated by $(1, 5)$ and $N = 23$ is suitable to identify the main effects for the model $\{(1,0), (2,0), (0,1), (0,2), (1, \pm 1), (1, \pm 2), (2, \pm 1), (2, \pm 2)\}$, but not the interactions since for example the frequencies $(1, 2)$ and $(2, 2)$ are aliased, being both in $L_{11}^\perp \cup L_{-11}^\perp$. The following theorem summarises this.

Theorem 35 *Let the set $A^+ = \{h_k \in \mathbb{Z}^d : k = 1, \dots, m\}$ define a Fourier model. Consider the lattice design $L_{g,N}$ and let N be odd. The Fourier model A^+ is identifiable by $L_{g,N}$ if and only if for every $k = 0, \dots, \frac{N-1}{2}$ there exists at most one $h_k \in A^+$ such that*

$$h_k^t g \equiv k \pmod{N} \quad \text{or} \quad h_k^t g \equiv -k \pmod{N}.$$

In particular $m \leq \frac{N-1}{2}$.

Since Fourier models always contain the constant term θ_0 (α_0) we are only considering $h_1, h_2 \notin L^\perp$ since any $h \in L^\perp$ will be aliased with the constant term. The theory can be adjusted to the case with a missing constant term (see Schwabe, 1994 [65]).

5.6 Orthogonality of multirank lattices for Fourier models

In this section we study the orthogonality of multirank lattice designs for Fourier models. From Subsection 4.3.1 recall the definition of lattices with more than one generator, Theorem 20 and Lemma 2 of Section 4.3.

Definition 31 *A lattice design of rank r is a uniform design supported over a lattice of rank r . The lattice design of rank r generated by g_1, \dots, g_r and with invariants N_1, \dots, N_r is represented by $L_{(g_1, \dots, g_r), \{N_1, \dots, N_r\}}$.*

One-generator lattice designs are lattice designs of rank 1. Exactly as in the one-generator case one can show that the following is true.

Theorem 36 *A lattice design (of rank r) is orthogonal for a Fourier model generated by A if and only if for all h_1 and h_2 ($h_1 \neq h_2$) frequencies in A the vectors $h_1 + h_2$, h_1 and h_2 do not belong to L^\perp . For $h_1, h_2 \in A^+$, where A^+ is minimal with respect to inclusion and $A = A^+ \cup \{-A^+\} \cup \{0\}$ this becomes $h_1, h_2, h_1 \pm h_2 \notin L^\perp$.*

Theorem 37 *Let L be a rank 2 lattice generated by g_1, N_1 and g_2, N_2 . Then $(a, b) \in L^\perp$ if and only if $(a, b)^t g_1 \in N_1 \mathbb{Z}$ and $(a, b)^t g_2 \in N_2 \mathbb{Z}$.*

Proof. Recall that

$$L^\perp = \left\{ g \in \mathbb{Z}^2 : h^t x \in \mathbb{Z} \text{ for all } x \in L \right\}.$$

If $(a, b)^t g_1 \in N_1 \mathbb{Z}$ and $(a, b)^t g_2 \in N_2 \mathbb{Z}$, then clearly $(a, b) \in L^\perp$. Let N be $N_1 N_2$. By definition $(a, b) \in L^\perp$ if and only if $\frac{1}{N} (a, b)^t (k g_1 + h g_2) \pmod{N} \in \mathbb{Z}$ for all $k, h = 0, \dots, N-1$, or $(a, b)^t (k g_1 + h g_2) \in N \mathbb{Z}$ for all $k, h = 0, \dots, N-1$. That is $(a, b)^t k g_1 + (a, b)^t h g_2 \in N \mathbb{Z}$ for all $k, h = 0, \dots, N-1$. For $k = 0$ we have $(a, b)^t g_2 \in N_2 \mathbb{Z}$ and for $h = 0$ we have $(a, b)^t g_1 \in N_1 \mathbb{Z}$. ■

Let us consider as an example the two-dimensional design supported on the rank 2 lattice generated by $g_1 = (2, 0)$, $N_1 = 4$ and $g_2 = (1, 1)$, $N_2 = 4$ according to Theorem 20. So that

$$L = \left\{ \frac{a(2,0)+b(1,1)}{4} : a, b = 0, 1, 2, 3 \right\} \quad M_l = \begin{pmatrix} \frac{1}{2} & 0 \\ \frac{1}{4} & \frac{1}{4} \end{pmatrix}$$

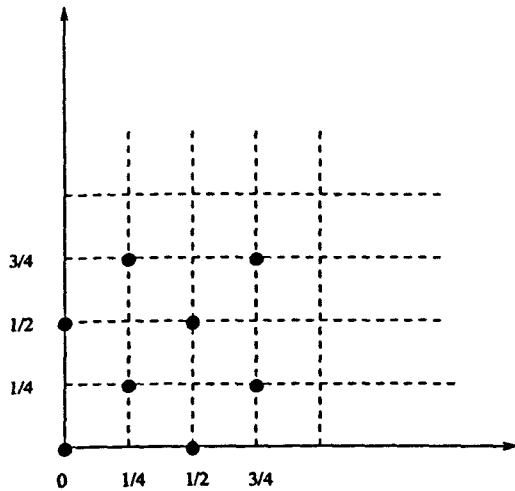


Figure 5.1: Lattice generated by $g_1 = (2, 0)$, $N_1 = 2$ and $g_2 = (1, 1)$, $N_2 = 4$.

gives the 8-point design $(0, 0), (1, 1), (2, 2), (3, 3), (2, 0), (3, 1), (0, 2), (1, 3)$ shown in Figure 5.1, which is the union of two 2^2 full-factorial one at levels 0 and $\frac{1}{2}$ and the other one at levels $\frac{1}{4}$ and $\frac{3}{4}$. The dual lattice is generated by $(M_L^{-1})^t$ that is

$$M_{L^\perp} = \begin{pmatrix} 2 & -2 \\ 0 & 4 \end{pmatrix}.$$

By analogy to the one-generator case we say that two frequencies h_1 and h_2 are mutually orthogonal with respect to L if and only if $h_1 \pm h_2 \notin L^\perp$, $h_1 \notin L^\perp$ and $h_2 \notin L^\perp$. Note that without loss of generality we can choose frequencies from the following set

$$\{(k, h) : k, h = 0, \dots, 3\} \setminus \{(0, 0)\}$$

that has 15 elements. Indeed we can easily find and eliminate the frequencies h such that $h \in L^\perp$ and those for which $2h \in L^\perp$ (note we have to impose explicitly $2h_1 \notin L^\perp$ since $N_2 = 4$ is even). Imposing the condition $h_1 \pm h_2 \notin L^\perp$ for $h_1 \neq h_2$ the set of possible frequencies is reduced to

$$A^+ := \{(0, 1), (1, 0)\}.$$

The set A^+ is actually of mutually orthogonal frequencies and thus it defines a Fourier model identifiable by L . For example the frequencies $(1, 2)$ and $(3, 2)$ belong to the same aliasing class since $(1, 2) + (3, 2) = (0, 0) \pmod{4}$. It is also maximal in the sense that any other frequency is not mutually orthogonal with at least one of the elements of A^+ . The estimable model found is not saturated while the one-generator lattice $L_{(1,2),5}$ identifies it with a minimum sample size.

As another example consider the 3-dimensional lattice of rank 2 generated by $g_1 = (1, 2, 5)$ with $N_1 = 9$ and $g_2 = (3, 5, 11)$ with $N_2 = 3$. Notice that g_2 can be substituted by $g_2 = (0, 2, 2)$. The design has 27 points. Thus we are able to identify at most 13 frequencies. The identifiable frequencies must not be solutions of the

following system of equations

$$\begin{cases} a + 2b + 5c \equiv 0 \pmod{9} \\ b + c \equiv 0 \pmod{3} \end{cases} \quad (5.2)$$

derived from $h^t g_1 \equiv 0 \pmod{9}$ and $h^t g_2 \equiv 0 \pmod{3}$. From Equations (5.2) we see that a subset of any possible set of identifiable frequencies is of the form $h = (a, b, c)$ where $b, c = 0, 1, 2$ and $a = 0, \dots, 8$. Imposing the conditions $h_1 \pm h_2 \notin L^\perp$ we find the following saturated set of identifiable frequencies

$$\{(1, 0, 0), (0, 1, 0), (0, 0, 1), (1, 1, 0), (1, 0, 1), (0, 1, 1), (1, 1, 1), \\ (2, 0, 0), (0, 2, 0), (0, 0, 2), (2, 1, 0), (2, 0, 1), (0, 2, 1)\}.$$

Theorem 38 *Let L be a d -dimensional lattice of rank r generated by g_1, \dots, g_r and with invariants N_1, \dots, N_r . The vector $h = (h_1, \dots, h_d) \in L^\perp$ if and only if it solves the following system of equations in \mathbb{Z}^d*

$$\begin{cases} h^t g_1 \equiv_{N_1} 0 \\ \vdots \\ h^t g_r \equiv_{N_r} 0. \end{cases}$$

Proof. The vector h is in L^\perp if the scalar product $h^t x \in \mathbb{Z}$ for all $x \in L$, that is for all vectors x of the form

$$\left\{ p_1 \frac{g_1}{N_1} + \dots + p_r \frac{g_r}{N_r} \right\} \quad \text{for } 0 \leq p_k \leq N_k \text{ for all } k = 1, \dots, r,$$

where as usual $\{a\}$ is the fractional part of a . If h satisfies the system then $h^t x \in \mathbb{Z}$.

Since the N_k must be such that N_{k+1} divides N_k for all $k = 1, \dots, r-1$ we can define the integers $t_k = \frac{N_1}{N_k}$ for all $k = 2, \dots, r$ so that

$$x = \left\{ \frac{p_1 g_1 + p_2 t_2 g_2 \dots + p_r t_r g_r}{N_1} \right\}.$$

The condition $h^t x \in \mathbb{Z}$ for all $x \in L$ becomes $h^t (p_1 g_1 + p_2 t_2 g_2 \dots + p_r t_r g_r) \in N_1 \mathbb{Z}$ for all $0 \leq p_k \leq N_k$, $k = 1, \dots, r$. In particular for $p_1 = 1$ and $p_k = 0$ for all $k = 2, \dots, r$ we have $h^t g_1 \equiv_{N_1} 0$. For $p_1 = 0$, $p_2 = 1$ and $p_k = 0$ for all $k = 3, \dots, r$ we have $h^t t_2 g_2 \in N_1 \mathbb{Z}$ that is $h^t g_2 \in N_2 \mathbb{Z}$. Analogously we determine the other equations of the required system. ■

Summary

In this chapter we give rules to determine complete Fourier models for which a given lattice design is orthogonal. These rules follow from a generalisation to lattices of the basic fact that the sum over the roots of unity of sine and cosine is zero (see Lemma 2). It turns out that the so-called dual lattice is important in describing the aliasing structure via a use of the cosets in the underlying cyclic group structure. There is a close connection with Nyquist sampling theory and Nyquist folding. The work can be considered as a generalisation of this theory from one dimension to multi-dimensional lattices.

Chapter 6

Finding good generators

Chapters 5 and 4 can be considered as a foundation for a more difficult problem: given a model, specified by a set of frequencies A , find a generator $g = (g_1, \dots, g_d)$ and a sample size N for which the orthogonality conditions in Chapter 5 hold. It will then work out that certain models, for example without high-order cross frequencies can lead to designs (generators) for which the sample size N only grows polynomially or even linearly in the dimension d . This points to a complexity theory for the design model pair (A, D) . Let us put this more precisely: what is the smallest sample size N^* such that there exists a generator g^* with $D = L_{g^*, N^*}$ satisfying the orthogonality conditions of Chapter 5? In many cases it appears that N^* is hard to find explicitly and we shall find $L_{g, N}$ with a suitable upper bound $N \geq N^*$.

Let $K(A)$ be some measure of the size of the model A such as the total number of frequencies or the order of the model. Since N^* represents a broad measure of the sampling density and $K(A)$ will typically measure quantities such as the largest fitted frequency or the number of distinct frequencies, the result can be thought of a kind of Nyquist-Shannon sampling theory. See in particular Section 6.2.

We consider certain classes of complete models, for example the two-factor interaction models with equal order of the marginals, $F(d; m, \dots, m; 2)$ and look for classes of generators, (g_1, \dots, g_d) and sample sizes, N_d such that the resulting lattices are orthogonal for the given models. We determine generators such that the sample size increases polynomially as the dimension increases. In Section 6.1 we describe the prototypes of generators we are interested in. In Section 6.2 we give rules for suitable sample sizes, the generator sequence being known. In Section 6.3 and 6.4 we present some examples.

6.1 Generator prototypes

Since the first order frequencies in each factor are present in all the Fourier models we treat, the entries g_1, \dots, g_d of a generator (g_1, \dots, g_d) have to be different. Without loss of generality we suppose $1 = g_1 < \dots < g_d$ (see Assumptions 2 and 3). If needed one rearranges the factors. We use the following types of generators: (i) power generator and generalised power generator

$$(g_1, \dots, g_d) = (1, p_1, p_1 p_2, \dots, \prod_{k=1}^{d-1} p_k)$$

where p_k are defined case by case; (ii) automatic or Fibonacci type generator; (iii) linear generator; (iv) one-step generator which considers as the next generator the smallest integer such that the conditions of Section 5.3 are satisfied.

Automatic rules are derived as two or three term non-homogeneous linear recursion formulae for the generator sequences such that the conditions in the suitable theorem of Section 5.3 hold in \mathbb{Z} . Typically they will be expressions of the form

$$\begin{aligned} g_0 &= g_0 \\ g_1 &= g_1 \\ g_d &= ag_{d-1} + bg_{d-2} + c \quad a, b, c \in \mathbb{R}. \end{aligned}$$

By the following theorem (see for example Biggs, 1994 [9]) we can express the g_d obtained by the recursive procedure in close form and thus conclude on the asymptotic behaviour of the generator sequence (and of the sample size) as the dimension increases.

Theorem 39 *Let g_d satisfy the following recursion scheme*

$$\begin{aligned} g_0 &= g_0 \\ g_1 &= g_1 \\ g_d &= ag_{d-1} + bg_{d-2} \end{aligned}$$

where $a, b \in \mathbb{R}$. Let α, β be the roots (real or imaginary) of the auxiliary equation

$$t^2 = at + b.$$

If $\alpha \neq \beta$ then there exist A and B real constant such that

$$g_d = A\alpha^d + B\beta^d \quad (6.1)$$

and if $\alpha = \beta$ then there exist A and B such that

$$g_d = (Ad + B)\alpha^d. \quad (6.2)$$

Proof. Let us suppose that Equations (6.1) and (6.2) hold. Then A and B are defined by the following identities

$$\begin{aligned} g_0 &= A + B & \text{or} & & g_0 &= B \\ g_1 &= A\alpha + B\beta & & & g_1 &= (A + B)\alpha. \end{aligned}$$

That Equations (6.1) and (6.2) hold is proved by induction on the dimension. We have just stated the theorem for $d = 0, 1$. First consider the case $\alpha \neq \beta$. By inductive hypothesis we have

$$g_d = A\alpha^d + B\beta^d.$$

The induction step is as follows. By definition we have

$$\begin{aligned} g_{d+1} &= ag_d + bg_{d-1} \\ &= a(A\alpha^d + B\beta^d) + b(A\alpha^{d-1} + B\beta^{d-1}) \\ &= A\alpha^{d-1}(a\alpha + b) + B\beta^{d-1}(a\beta + b) \\ &= A\alpha^{d+1} + B\beta^{d+1}. \end{aligned}$$

The last equality holds because α and β are roots of $t^2 = at + b$. If $\alpha = \beta$ we have

$$\begin{aligned} g_{d+1} &= a(Ad + B)\alpha^d + b(Ad + B)\alpha^{d-1} \\ &= Ad\alpha^{d-1}(a\alpha + b) + B\alpha^{d-1}(a\alpha + b) \\ &= Ad\alpha^{d+1} + B\alpha^{d+1} \\ &= (Ad + B)\alpha^{d+1}. \quad \blacksquare \end{aligned}$$

Lemma 3 *Let g satisfy*

$$\begin{aligned} g_0 &= g_0 \\ g_1 &= g_1 \\ g_d &= ag_{d-1} + bg_{d-2} + c \end{aligned} \quad (6.3)$$

then there exist $h_d \in \mathbb{R}$ and $p \in \mathbb{R}$ such that $g_d = h_d + p$ satisfies

$$\begin{aligned} h_0 &= g_0 - p \\ h_1 &= g_1 - p \\ h_d &= ah_{d-1} + bh_{d-2}. \end{aligned}$$

Proof. For $p = \frac{c}{1-a-b}$ the lemma holds. \blacksquare

As an example consider the following sequence

$$\begin{aligned} g_0 &= 1 \\ g_1 &= 3 \\ g_d &= 2g_{d-1} + g_{d-2} + 1 \end{aligned}$$

for which we have

$$g_d = \frac{3 + 2\sqrt{2}}{4}(1 + \sqrt{2})^d + \frac{3 - 2\sqrt{2}}{4}(1 - \sqrt{2})^d - \frac{1}{2}.$$

The Maple command `rsolve` implements the above procedure. For the above example we have the following

```
> A:=rsolve( {g(n) = 2*g(n-1)+g(n-2)+1, g(0)=1,g(1)=3},g(n) );
```

$$\begin{aligned} A := & -\frac{1}{2} \frac{\left(-\frac{1}{-\sqrt{2}+1}\right)^n}{-\sqrt{2}+1} - \frac{1}{2} \frac{\left(-\frac{1}{1+\sqrt{2}}\right)^n}{1+\sqrt{2}} - \frac{1}{2} \\ & + \frac{1}{8} \frac{(-2+\sqrt{2})\sqrt{2}\left(-\frac{1}{-\sqrt{2}+1}\right)^n}{-\sqrt{2}+1} + \frac{1}{8} \frac{\sqrt{2}(2+\sqrt{2})\left(-\frac{1}{1+\sqrt{2}}\right)^n}{1+\sqrt{2}} \end{aligned}$$

```
> simplify(A*(-1+sqrt(2))*(1+sqrt(2))*(-1+sqrt(2))^(n*(1+sqrt(2)))^n);
```

$$\frac{3}{4} (1 + \sqrt{2})^n + \frac{1}{2} (1 + \sqrt{2})^n \sqrt{2} - \frac{1}{2} \sqrt{2} (-\sqrt{2} + 1)^n + \frac{3}{4} (-\sqrt{2} + 1)^n - \frac{1}{2}$$

The second command was needed to obtain a neater form of the result.

Another approach to the study of recursive sequences of generators is based on generating functions and exponential generating functions. We refer to the book by Herbert S. Wilf (1990) [75].

Definition 32 *The generating function of the sequence $\{g_n\}$ is the analytic function (if any) to which the power series*

$$F(t) = \sum_{n=0}^{+\infty} g_n t^n$$

converges in a suitable interval of $t = 0$.

Wilf (1990) [75] shows how generating functions are useful not only to study the asymptotic behaviour of sequences but also to determine the average of a given sequence such as $\frac{F'(1)}{F(1)}$ (if $F(1)$ and $F'(1)$ exist) and other statistical properties. Since the sequences we are interested in assume integer values, $g_d \in \mathbb{Z}_+$ for all d , the generating function of a lattice-generator sequence does never converge at 1.

Next we show a method to find generating functions with the help of the above sequence. Let us formally write $F(t) = \sum_{d=0}^{+\infty} g_d t^d$ and consider the following steps

$$\begin{aligned} t^d g_d &= 2t^d g_{d-1} + t^d g_{d-2} + t^d \\ \sum_{d=2}^{+\infty} t^d g_d &= 2t \sum_{d=2}^{+\infty} t^{d-1} g_{d-1} + t^2 \sum_{d=2}^{+\infty} t^{d-2} g_{d-2} + \sum_{d=2}^{+\infty} t^d \\ F(t) - t g_1 - g_0 &= 2t(F(t) - g_0) t^2 F(t) + \frac{1}{1-t} - 1 - t. \end{aligned}$$

Since we are operating formally we ignore the fact that $\sum_{d=0}^{+\infty} t^d$ converges to $\frac{1}{1-t}$ only for $|t| < 1$ and $t = -1$ and we have

$$\begin{aligned} F(t)(1 - 2t - t^2) &= \frac{1}{1-t} \\ F(t) &= \frac{1}{(1 - 2t - t^2)(1 - t)}. \end{aligned}$$

The denominator is formally equal to the auxiliary equation evaluated in $1/t$ and in particular $F(t)$ is defined over $\mathbb{R} \setminus \{-1 \pm \sqrt{2}, 1\}$. Then the convergence is absolute for t in the open interval $(-1 - \sqrt{2}, -1 + \sqrt{2})$.

In general the generating function of the sequence defined by Equations (6.3) is

$$F(t) = \frac{t^2(ag_0 - g_1 + c) + t(g_1 - g_0(a + 1)) + g_0}{(1 - at - bt^2)(1 - t)}.$$

Definition 33 *The exponential generating function of the sequence $\{g_n\}$ is, if exists,*

$$F(t) = \sum_{n=0}^{+\infty} \frac{g_n}{n!} t^n.$$

Exponential generating functions are useful when treating derivatives in particular let F be the exponential generating function of $\{g_n\}$ then $\frac{dF^h}{dt^h}$ is the exponential generating function of $\{g_{n+h}\}$. The exponential generating function for the above recursion is

$$G(t) = -\frac{e^t}{2} + \frac{1 + \sqrt{2}}{4} e^{(\sqrt{2}+1)t} + \frac{1 - \sqrt{2}}{4} e^{-(\sqrt{2}-1)t}$$

obtained as follows. First notice that

$$\begin{aligned} G(t) &= \sum_{n=0}^{+\infty} \frac{g_n}{n!} t^n \\ G'(t) &= \sum_{n=1}^{+\infty} \frac{g_n}{(n-1)!} t^{n-1} \\ G''(t) &= \sum_{n=2}^{+\infty} \frac{g_n}{(n-2)!} t^{n-2}. \end{aligned}$$

Next multiplying the above recursion scheme by $\frac{t^{n-2}}{(n-2)!}$ and summing over n we have

$$\sum_{n=2}^{+\infty} \frac{g_n}{(n-2)!} t^{n-2} = 2 \sum_{n=2}^{+\infty} \frac{g_{n-1}}{(n-2)!} t^{n-2} + \sum_{n=2}^{+\infty} \frac{g_{n-2}}{(n-2)!} t^{n-2} + \sum_{n=2}^{+\infty} \frac{1}{(n-2)!} t^{n-2}$$

which corresponds to the Cauchy problem

$$\begin{cases} G''(t) - 2G'(t) - G(t) = e^t \\ G(0) = g_0 = 1 \\ G'(0) = g_1 = 3 \end{cases}$$

whose solution leads to the above analytic form of $G(t)$.

Next we present an algorithm for an iterative sequence of generator components obtained by a *one-step* strategy. The one-step algorithm gives a reasonable bound on the increase of the generator components and, hence, of a suitable size as the dimension d increases.

For the generator (g_1, \dots, g_d) denote by $\mathcal{A}_d^{(M)}$ 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, $1 \leq S \leq M$, and that the generator (g_1, \dots, 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 to each other (within the set \mathbb{Z} of all integers). Then $\mathcal{A}_d^{(S)}$ is the set that collects the members of the first $S+1$ rows of the array and, in particular, $\mathcal{A}_d^{(0)} = \{0\}$.

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

$$\mathcal{A}_1^{(S)} = \{-m_1, \dots, -1, 0, 1, \dots, m_1\}, \quad 1 \leq S \leq M.$$

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

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

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 in all factors, the constructions in the algorithm guarantee that $g_d = O(d^{M+S-1})$, as $d \rightarrow \infty$, because the cardinality of $\mathcal{A}_d^{(S)}$ increases like $O(d^S)$ and hence the cardinality of \mathcal{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 \mathcal{A}_d^{++} the iterative sequence of generator components and the corresponding sizes increase polynomially. This is to be compared to exponential growth for 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 .

Finally we present a methodology from computer algebra and specifically Gröbner bases for the one-step algorithm. The nicest feature of this approach is that it does not require the generators to be an increasing sequence. First note that the conditions to be checked from Theorem 26 are the complement of linear algebraic varieties. This is made clear by an example. Consider the model $F(2; 4, 2; 1)$. The array to be checked to ensure that the design generated by $g = (g_1, g_2) \in \mathbb{Z}_+^2$ is orthogonal for such a model reduces to the occurrence of the following inequalities

$$g_1 \neq \pm g_2, 2g_1 \neq \pm g_2, 3g_1 \neq g_2, 4g_1 \neq g_2, g_1 \neq 2g_2, 3g_1 \neq 2g_2.$$

The set of (g_1, g_2) satisfying these conditions is the complementary set in for example \mathbb{Z}_+^2 of the following union of varieties

$$V = V(g_1^2 - g_2^2) \cup V(2g_1^2 - g_2^2) \cup V(3g_1^2 - g_2^2) \cup V(4g_1^2 - g_2^2) \cup V(g_1^2 - 2g_2^2) \cup V(3g_1^2 - 2g_2^2).$$

A basis for the ideal $I(V)$ corresponding to this variety is the following polynomial

$$p = (g_1^2 - g_2^2)(2g_1^2 - g_2^2)(3g_1^2 - g_2^2)(4g_1^2 - g_2^2)(g_1^2 - 2g_2^2)(3g_1^2 - 2g_2^2).$$

We then require that a good generator (\hat{g}_1, \hat{g}_2) does not belong to V . Consider the polynomial system corresponding to the generator

$$\begin{cases} p_1 = g_1 - \hat{g}_1 = 0 \\ p_2 = g_2 - \hat{g}_2 = 0. \end{cases}$$

By the ideal membership theorem (Theorem 10 in Section 2.3) we require that the remainder of p by the Gröbner basis generated by p_1 and p_2 is non zero, specifically a non zero constant. It is a constant since p_1 is of first degree in g_1 and p_2 is of first degree in g_2 . By substituting $g_1 = 1$ we require that g_2 should not take any of the following values

$$\pm 1, \pm 2, \pm 3, \pm 3, \pm 4, \pm \frac{1}{2}, \pm \frac{3}{2}.$$

As another example consider the Fourier model $F(3; 1, 1, 1; 1)$. The conditions to be checked correspond to the ideal generated by the following polynomial

$$p = (g_2 - g_1)(g_1 + g_2)(g_2 - g_3)(g_2 + g_3)(g_1 - g_3)(g_1 + g_3).$$

We choose $g_1 = 1, g_2 = 5$ and want to determine a value c for g_3 . The polynomial system for the generator is as follows

$$\begin{cases} p_1 = g_1 - 1 = 0 \\ p_2 = g_2 - 5 = 0 \\ p_3 = g_3 - c = 0. \end{cases}$$

It is a Gröbner basis since it is formed of linear polynomials. The remainder of the division of p by p_1, p_2, p_3 is $600 - 624c^2 + 24c^4$. Its factorisation in irreducible factors is $(c - 1)(c - 5)(c + 5)(c + 1)$ from which we deduce that any c different from ± 1 and ± 5 is a suitable choice for g_3 . Notice that we could have considered only the "positive" conditions that is $g_1 \neq g_2, g_1 \neq g_3$ and $g_2 \neq g_3$. We consider the above an amusing note and discuss it no further.

6.2 Sample size

Given a generator, g we check whether all the entries in the suitable array in Theorem 26 are different in the set of all positive integers. If this holds then they are also different in the cyclic group \mathcal{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 different within the cyclic group \mathcal{G}_N . To reduce the size we can match the larger members of the array into suitable gaps in the upper half. Because of the symmetry of the array with respect to zero the corresponding negative members automatically fit into gaps in the lower half. Usually the largest gap is between the maximum member, N_1 , and the next to maximum one, say N_2 and in general $N_1 > N_2 + 1$. So a size $N_1 + N_2 + 1$ is suitable and gives a reduction of, at most, g_d . We refer to it with the term *Generalised 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_1 is the largest member in the whole array a straightforward *Generalised Upper Law for Main Effects* states that a size $N_1 + N_3 + 1$ is suitable. Notice that any size larger than the ones given by these laws is suitable.

Let us comment again on the choice of N and its link to the Nyquist frequency as in Fourier Analysis. The Nyquist frequency in discrete Fourier Analysis is the highest frequency f^* used in Fourier transform. If Δt is the sampling interval in time, then $2\pi f^* = \frac{\pi}{\Delta t}$. For all the frequencies $f < f^*$ the components with frequencies $f + kf^*$ ($k \in \mathbb{Z}$) are all aliased with each other and the sum of their contributions appear collected, at frequency f . This is sometimes referred to as *Nyquist folding*. To avoid this the frequencies under study must be less than the Nyquist frequency, equivalently the sampling interval is chosen to make this happens. In other terms we require $2\pi f < \frac{\pi}{\Delta t}$. In the case of N equally spaced points Δt is $\frac{1}{N}$ and we have $2\pi f < \pi N$ that is $2f + 1 \leq N$. Here the largest member of the array in Theorem 26 plays the role of the Nyquist frequency. For example, as we shall see in Section 6.3 for the model $F(d; m, \dots, m; 1)$ a suitable sequence of generator is given by

$$\begin{aligned} g_1 &= 1 \\ g_k &= (d - 1)m + 1 \quad \text{for all } k = 2, \dots, d \end{aligned}$$

with a sample size of $N = 2m^2(d - 1) + 2m + 1$. The quantity $m^2(d - 1) + m$ represents the Nyquist frequency. It is also suitable as $K(A)$ in the discussion at the beginning of this chapter.

The examples in the next sections are accompanied by a series of tables. The legend in the tables is as follows: "Dim" stands for "dimension", "gen" for "generator", N_1 is the largest number and N_2 is the second-largest number in the array to be checked. By UL we mean the number of supporting points given by the *Upper Law* and Gen UL by the *Generalised Upper Law*. Finally "Min.Size" is the minimum number of supporting points for the generator in the row.

We recall from Section 5.2 and Section 4.2 that for the complete model, $F(d; m_1, \dots, m_d; d)$ the uniform design supported on the integer grid

$$\left\{ \left(\frac{k_1}{m_1}, \dots, \frac{k_d}{m_d} \right) : k_1 = 0, \dots, 2m_1, \dots, k_d = 0, \dots, 2m_d \right\}$$

is orthogonal with a minimal sample size $\prod_{k=1}^d (2m_k + 1)$. It is also a lattice design generated by the generalised power generator

$$(g_1, \dots, g_d) = (1, p_1, p_1 p_2, \dots, \prod_{i=1}^{d-1} p_i)$$

where $p_i = 2m_i + 1$. Moreover the above design is orthogonal for any submodel of the complete model, that is for $F(d; m_1, \dots, m_d; M)$ where $M < d$. However, the number of design points is, in general, much larger than the number of parameters. In Section 6.3 we consider alternative lattice designs for linear models.

6.3 Additive models

According to Theorem 29 a lattice design with generator $g = (g_1, \dots, g_d)$ and a sample size N is orthogonal for the additive model $F(d; m_1, \dots, m_d; 1)$ if and only if the entries in the following array are all different modulo N

$$0, g_k h_k : h_k = \pm 1, \dots, \pm m_k \quad k = 1, \dots, d. \quad (6.4)$$

6.3.1 Power type generators

Since $F(d; m_1, \dots, m_d; 1)$ is a submodel of $F(d; m_1, \dots, m_d; d)$ the generalised power generator of the Section 6.2 with a sample size $N = \prod_{k=1}^d (2m_k + 1)$ is suitable. By the Upper law the sample size can be reduced to $N = 2m_d \prod_{k=1}^{d-1} (2m_k + 1) + 1$. In the case of equal order marginals, $m_k = m$ for all $k = 1, \dots, d$ it becomes $N = 2m(2m + 1)^{d-1} + 1$ which increases exponentially in the dimension while the number of parameters, $1 + 2dm$ increases linearly.

We notice that in the array there is a considerable gap at the start between m and $2m + 1$ and suggest the *power generator* with minimum base $m + 1$

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

Theorem 40 For the model $F(d; m, \dots, m; 1)$ the power generator sequence

$$\begin{aligned} g_1 &= 1 \\ g_d &= (m + 1)^{d-1} \end{aligned}$$

with $N = 2m(m+1)^{d-1} + 1$ gives an orthogonal design.

Proof. The array to be checked becomes

$$0, \\ h_k(m+1)^{k-1}, \quad h_k = -m, \dots, m, \quad k = 1, \dots, d.$$

The positive entries of the array are different from each other in \mathbb{Z} since for all k

$$\begin{array}{ll} h_k(m+1)^{k-1} < h_l(m+1)^{k-1} & \text{for all } h_k < h_l \quad \text{and} \\ mg_k < g_{k+1} & \text{since } m(m+1)^{k-1} < (m+1)^k. \end{array}$$

The biggest of these positive entries is $m(m+1)^{d-1}$ which is smaller than $N/2$. This implies that every negative entry of the array (mod N) is bigger than any positive entry. This proves the assert. ■

The size $N = 2m(m+1)^{d-1} + 1$ given by the *Upper Law* is approximately $1/2^{d-1}$ times the size for the power generator with base $2m+1$ but still increases exponentially with the dimension.

The following general result is proved analogously to Theorem 40.

Theorem 41 For $F(d; m_1, \dots, m_d; 1)$ the generalised power generator

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

with a size $N = 2m_d \prod_{k=1}^{d-1} (m_k + 1) + 1$ is an orthogonal design.

6.3.2 Recursively defined generators

For the model $F(d; 1, \dots, 1; 1)$ the lattice design generated by

$$(g_1, \dots, g_d) = (1, 2, 3, \dots, d-1)$$

and with minimum sample size $2d-1$ is orthogonal. This suggests an iterative strategy for adding dimensions. Suppose the $(d-1)$ -dimensional generator (g_1, \dots, g_{d-1}) is such that the members of the array

$$0, \\ r_k g_k \quad r_k \in \mathcal{N}_k^*, \quad k = 1, \dots, d-1$$

are distinct in \mathbb{Z} , then we choose the next generator g_d greater than the largest member of the above array. The resulting generator (g_1, \dots, g_d) produces an array in which again all members are distinct. The largest member at each step will be $m_d g_d$ such that $g_d \geq m_{d-1} g_{d-1} + 1$. As we want to choose g_d as small as possible in order to reduce the gaps in the array we obtain the following recursion scheme

$$\begin{array}{l} g_1 = 1 \\ g_d = m_{d-1} g_{d-1} + 1 \end{array}$$

and a size $2m_d g_d + 1$ by the *Upper Law*. This leads to the next theorem.

Theorem 42 For the model $F(d; m_1, \dots, m_d; 1)$ the recursive scheme

$$\begin{aligned} g_1 &= 1 \\ g_d &= m_{d-1}g_{d-1} + 1 \end{aligned}$$

and $N = 2m_d g_d + 1$ give an orthogonal design.

Proof. From the following identity

$$\begin{aligned} g_1 &= 1 \\ g_d &= \sum_{l=1}^{d-1} \prod_{k=l}^{d-1} m_k + 1 \end{aligned}$$

we deduce that the positive entries of the Array (6.4) are distinct in \mathbb{Z} . The negative entries of the Array (6.4) (mod $N = 2m_d g_d + 1$) are greater than $\sum_{i=1}^d m_i$ since the number of positive entries is $\sum_{i=1}^d m_i$ which is smaller than $N/2$. This concludes the proof. ■

The sample size in Theorem 42 is smaller than the sample size of the power generator design but still increases exponentially with the dimension. In fact for $m_1 = \dots = m_d = m$ we have

$$g_d = \frac{m^d - 1}{m - 1} \quad \text{and} \quad N = 2m \frac{m^d - 1}{m - 1} + 1$$

To improve upon this we arrange the model factors in such a way that $m_1 \geq m_2 \geq \dots \geq m_d$. The recursive procedure

$$\begin{aligned} g_1 &= 1 \\ g_d &= (d - 1)m_1 + 1 \end{aligned}$$

and $N = 2m_1^2(d - 1) + 2m_1 + 1 \geq 2 \max_{k=1, \dots, d} \{g_k m_k\} + 1$ give a design whose size increases linearly with the dimension when the orders m_k remain bounded. Note that a new rearrangement of the factors has to be made each time a new factor is added. This is summarised in the following theorem

Theorem 43 For the model $F(d; m_1, \dots, m_d; 1)$ where $m_1 \geq m_2 \geq \dots \geq m_d$ the recursive scheme

$$\begin{aligned} g_1 &= 1 \\ g_d &= (d - 1)m_1 + 1 \end{aligned}$$

and $N = 2m_1^2(d - 1) + 2m_1 + 1$ give an orthogonal design whose sample size increases linearly in the dimension.

For the model $F(d; 2, \dots, 2; 1)$ Theorem 43 gives the first d odd numbers (including one) as generator sequence and a sample size $N = 8d - 3$.

Tables 6.4, 6.5 and 6.6 give the linear recursive sequence for the models $F(d; 2, \dots, 2; 1)$, $F(d; 3, \dots, 3; 1)$ and $F(d; 4, \dots, 4; 1)$ respectively. Let us see how we determined the minimum sample sizes for the one-step generator given in the tables.

Theorem 44 For the model $F(d; 2, \dots, 2; 1)$ and the generator sequence

$$g_d = 2d - 1$$

the minimum sample size is $4d + 2$.

Proof. The number of parameters, $4d + 1$ is a lower bound for the sample size. The minimum size cannot be $N = 4d + 1$ otherwise $2g_d = -3 \pmod{N}$. It remains to show that all the numbers in

$$0, \pm g_k \pmod{4d + 2}, \pm 2g_k \pmod{4d + 2}: \quad k = 1, \dots, d$$

are distinct. The following holds

$$\begin{aligned} 0 &\equiv 0 \pmod{4d + 2} \\ g_k &\equiv 2k - 1 \pmod{4d + 2} \equiv \begin{cases} 1 & \text{if } k \text{ is odd} \\ 3 & \text{if } k \text{ is even} \end{cases} \pmod{4} \quad k = 1, \dots, d \\ -g_k &\equiv 4d - 2k + 3 \pmod{4d + 2} \equiv \begin{cases} 1 & \text{if } k \text{ is even} \\ 3 & \text{if } k \text{ is odd} \end{cases} \pmod{4} \quad k = 1, \dots, d \\ 2g_k &\equiv 4k - 2 \pmod{4d + 2} \equiv 2 \pmod{4} \quad k = 1, \dots, d \\ -2g_k &\equiv 4(d - k) + 4 \pmod{4d + 2} \equiv 0 \pmod{4} \quad k = 1, \dots, d. \end{aligned}$$

The numbers in each lines are clearly all different from each other. Since $g_k < \frac{4d+2}{2}$, $-g_k \pmod{N}$ is bigger than g_l for all k and l in $\{1, \dots, d\}$. The other numbers belonging to different lines are different from each other because they are different $\pmod{4}$ (the first and the last line are considered together). ■

Theorem 45 Let $d > 2$. For the model $F(d; 3, \dots, 3; 1)$ and the generator sequence

$$g_d = 3d - 2$$

the minimum sample size is $9d$.

Proof. The lower bound given by the number of parameters is $6d + 1$. The lower bound can be improved to $9d - 1$. This is because the sample size cannot be $N = 9d - 5, 9d - 4, 9d - 3, 9d - 2$ or $9d - 1$ because otherwise the $-1, -2, 3$ or -4 would be equal to $9d - 6$ which belongs to the array to be checked. It cannot be less then $9d - 6$ because of the shapes of the holes left by the positive entries in the array to be filled in by the negative entries \pmod{N} . Indeed the positive part of the array for $d = 13$ has the following form

1	4	7	10	13	16	19	22	25	28	31	34	■
2		8		14		20		26		32		■
3			12			21			30			■
37	/	/	/	/	/	/	/	/	/	/	/	■
38		44		50		56		62		68		■
39			48			57			66			■
74	/	/	/	/	/	/	/	/	/	/	/	■
75			84			93			102			111

where all the positions in the first row, alternate position in the second row and one out of three in the third row are occupied. A symbol “/” is used for a position that will be occupied if we were in dimension higher than 13. In particular the shapes of the holes left up to 39 is recursively repeated increasing the dimension.

The rest of the proof follows closely that of Theorem 44. We have to show that the size of the following set is $9d$

$$0, \pm g_k \pmod{9d}, \pm 2g_k \pmod{9d}, \pm 3g_k \pmod{9d} : k = 1, \dots, d.$$

The following holds

$$\begin{aligned} 0 &\equiv 0 \pmod{9d} \\ g_k &\equiv 3k - 2 \pmod{9d} \equiv 1 \pmod{3} & k = 1, \dots, d \\ 2g_k &\equiv 6k - 4 \pmod{9d} \equiv 2 \pmod{3} & k = 1, \dots, d \\ 3g_k &\equiv 9k - 6 \pmod{9d} \equiv 0 \pmod{3} & k = 1, \dots, d \\ -g_k &\equiv 9d - 3k + 2 \pmod{9d} \equiv 2 \pmod{3} & k = 1, \dots, d \\ -2g_k &\equiv 9d - 6k + 4 \pmod{9d} \equiv 1 \pmod{3} & k = 1, \dots, d \\ -3g_k &\equiv 9d - 9k + 6 \pmod{9d} \equiv 0 \pmod{3} & k = 1, \dots, d. \end{aligned}$$

The numbers in each lines are clearly distinct. Values belonging to the first three lines are different from each other because they assume different values (mod 3). The same holds for number in the last three lines. Thus we are left to prove that for all k, l the following three inequalities hold

$$\begin{aligned} 2g_k &\neq -g_l \pmod{9d} \\ 3g_k &\neq -3g_l \pmod{9d}. \end{aligned}$$

From $2g_k = -g_l$ we get $3(2k + 2l - 3da) = 8$, for some integer a , which is impossible. From $3g_k = -3g_l$ we get $3(k + l - da) = 4$, for some integer a , which is impossible. This proves the assertion. ■

Theorem 46 *Let $d > 2$. For the model $F(d; 4, \dots, 4; 1)$ and the generator sequence*

$$g_d = 4d - 3$$

the minimum sample size is $16d - 6$.

Proof. The proof is similar to that of Theorem 45. We only sketch it here. For $d = 5$ the array has the following shape

1	5	9	13	17	/	/	/	/	/	/	/	/	/	/
2		10		18	26	34	/	/	/	/	/	/	/	/
3			15		27	39		51		/				
4				20		36		52					68	

from which we deduce that a minimum sample size must be larger than the largest element in the array, that is $4(4d - 3)$. An exhaustive search shows that the integers between $16d - 11$ and $16d - 5$ are not suitable. Finally $N = 16d - 6$ is found to be suitable. For example for $d = 5$ the opposite (mod N) of the largest member of the array, that is 68, becomes 7 and again the shape of the holes left allows us to fold the negative entries of the array suitably and thus complete the proof. ■

6.3.3 One-step generators and linear generators

Next we present the iterative *one-step strategy* for additive models. By this strategy given a $(d - 1)$ -dimensional generator (g_1, \dots, g_{d-1}) such that the members of the array

$$0, \\ r_k g_k \quad r_k \in \mathcal{N}_k^*, \quad k = 1, \dots, d - 1$$

are distinct in \mathbb{Z} we choose the next generator g_d as the smallest integer such that when we add

$$r_d g_d \quad r_d \in \mathcal{N}_d^*,$$

the increased array has still all members distinct in \mathbb{Z} . In Table 6.1 there is the code of the one-step strategy algorithm for the additive case. We use the language for computer algebra CoCoAL because of its flexibility in managing sets and lists. From this code we had the results in Tables 6.7, 6.8 and 6.9. The entries in the last column of these three tables have been entered by exhaustive search.

Theorem 47 *For the model $F(2; m, m; 1)$ the linear generator $(1, m + 1)$ is also the one-step generator. By the Upper Law the size is $2m^2 + 2m + 1$ and by the Generalized Upper Law it is $2m^2 + m$. A complete compression gives $m^2 + 2m + 2$.*

Proof. A minimal sample size, N cannot be smaller than $m^2 + 2m$. Indeed let N be strictly smaller than $m^2 + 2m$ then by the integer division there exist $0 \leq \beta \leq m$ and $1 \leq \alpha \leq m$ such that $N = \alpha(m + 1) + \beta$ and thus $\alpha(m + 1) = -\beta \pmod{N}$ but both belong to the array to be checked. It neither can be $N = m^2 + 2m + 1$ otherwise $m + 1 = -m(m + 1) \pmod{N}$. The next integer $N = m^2 + 2m + 2$ is suitable. Indeed we can organise the positive entries of the array to be checked in a table as follows

1	$m + 1$	$2(m + 1)$	\dots	$m(m + 1)$
2				
3				
\vdots				
$m - 1$				
m				

The opposites \pmod{N} of the numbers in the first column fill the last column of the above array and the opposites \pmod{N} of the first row fill the second row, thus they are all distinct. ■

6.4 Two-factor interaction models

By Theorem 29 a generator g and a size N give an orthogonal design for the models $F(d; m_1, \dots, m_d; 2)$ if and only if the entries of the following array are all different from each other \pmod{N}

$$0, \\ r_k g_k, \quad r_k \in \mathcal{N}_{m_k}^*, \quad k = 1, \dots, d \\ r_k g_k + r_\ell g_\ell, \quad r_k \in \mathcal{N}_{m_k}^*, r_\ell \in \mathcal{N}_{m_\ell}^*, \quad 1 \leq k < \ell \leq d.$$

```

/*****
One-step generator for additive models  $F(d; m_1, \dots, m_d; 1)$ 
*****/
-- Input: a vector M for the order of the marginals
-- Output: the list of generators Gen
Define OneStepLin(M)
D:=NumComps(M);
Gen:=[1];
Array:=[ K | K In 1..M[1] ];
B:=[ K | K In 1..(Last(Array)+1) ];
Candidates:=Diff(B,Array);
Dimen:=2;
While Dimen <= D Do
  Found:=False;
  While Found=False Do
    Tmp:=First(Candidates);
    Candidates:=Diff(Candidates,[Tmp]);
    V:=[ K Tmp | K In 1..M[Dimen] ];
    If InterList(Array,V)
    Then
      Append(Gen,Tmp);
      Array:=Concat(Array,V);
      Array:=Set(Array);
      B:=[ K | K In 1..(Last(Array)+1) ];
      Candidates:=Diff(B,Array);
      Found:=True;
      Dimen:=Dimen+1;
    Else
      Tmp:=Tmp+1;
    End;
  End;
End;
Return(Gen);
End;
/*****
InterList check if two lists have common elements
*****/
-- Input: two list
-- Output: FALSE if the intersection is not empty
--          TRUE if the intersection is empty
InterList(A,V):= EqSet(Diff(A,V),A);

```

Table 6.1: Code for the one-step strategy for $F(d; m_1, \dots, m_d; 1)$.

As $F(d; m_1, \dots, m_d; 2)$ is a submodel of the complete model the generalised power generator with $p_i = 2m_i + 1$ produces an orthogonal lattice design. The Upper Law gives a size

$$2(m_d g_d + m_{d-1} g_{d-1}) + 1 = \prod_{k=1}^{d-2} (2m_k + 1) [4m_d m_{d-1} + 2m_d + 2m_{d-1}] + 1$$

which is slightly smaller than the size for a product type design. When analysing only the main effect, the Generalised Upper Law for Main Effects gives the following sample size

$$2m_d g_d + m_{d-1} g_{d-1} + 1 = \prod_{k=1}^{d-2} (2m_k + 1) [4m_d m_{d-1} + 2m_d + m_{d-1}] + 1.$$

In the study of two-factor interaction models we distinguish between inference on main effects and inference on the whole parameter vector. In particular we concentrate on the following three classes of models $F(d; 1, \dots, 1; 2)$, $F(d; 2, \dots, 2; 2)$ and $F(d; m, \dots, m; 2)$.

6.4.1 The models $F(d; 1, \dots, 1; 2)$

Given the generator (g_1, \dots, g_d) we have to check the entries of the array

$$\begin{array}{l} 0, \\ g_k, -g_k \quad \quad \quad k = 1, \dots, d \\ g_k + g_\ell, g_k - g_\ell, -g_k + g_\ell, -g_k - g_\ell, \quad 1 \leq k < \ell \leq d. \end{array}$$

The largest element in the array is $N_1 = g_d + g_{d-1}$ and the largest element of the first two rows, associated to the main effects, is $N_3 = g_d$.

From Section 6.2 we know that a power generator for making inference on both the main effects and on the whole parameter vector is $(1, 3, \dots, 3^{d-1})$ with a sample size of $7 \cdot 3^{d-2} + 1$ and $8 \cdot 3^{d-2} + 1$ by the Generalised Upper Law for Main Effects and the Upper Law respectively. This is also the power generator with minimum base.

For inference on the all effect parameter vector the minimum size greater than the largest element in the array is $N = 4 \cdot 3^{d-2} + 1$. Indeed all the positive entries are equal to themselves and distinct (mod N) since the factorisation into prime factors of g_k involves only 3, the one of the form $g_k + g_l$ involves 3 and the prime factors of a power of 3 plus 1, that is 4, 10, 28, etc. and the one of the form $g_k - g_l$ involves 3 and the prime factors of a power of 3 minus one. The opposite (mod N) of the positive entries are all equal to 1 (mod 3) and thus distinct from the positive entries. They are distinct from each other since $-g_k \pmod{N} - 1$ is divisible by 4 while $-(g_k + g_l)$

(mod N) - 1 is not and for all $0 \leq l < k \leq d - 1$ we have that $\frac{-(g_k - g_l)(\text{mod } N) - 1}{3^l} \pmod{3} = 1$ while $\frac{-(g_k + g_l)(\text{mod } N) - 1}{3^l} \pmod{3} = 2$. Stronger compressions are possible.

Theorem 48 *An iterative sequence of generator components for the inference on the main effects is given by the recursion*

$$\begin{array}{l} g_1 = 1 \\ g_d = 2g_{d-1} + 1 = 2^d - 1, \quad d \geq 2 \end{array}$$

and the size defined by the Generalised Upper Law for Main Effects is $5 \cdot 2^{d-1} - 2$. It increases exponentially.

Proof. Clearly the g_k are different from each other and from their additive inverses. Moreover $g_h \pm g_k \neq g_l$ for all l, k, h since $2^h - 1 \pm (2^k - 1)$ is equivalent to zero (mod 2) and $2^l - 1$ is equivalent to one (mod 2). ■

The recursion of Theorem 48 is not suitable for identification of the whole parameter vector since for example $g_k + g_h = g_l - g_m$ for $k = 1, h = 2$ and $l = 3, m = 2$.

Theorem 49 *The sequence of the first odd numbers $g_d = 2d - 1$ with size $6d - 4$, by the Generalised Upper Law for Main Effects defines a lattice design suitable for the estimation of the main effect of the model $F(d; 1, \dots, 1; 2)$. This is also the one-step generator.*

Proof. The g_k are different from each others. For all k and all $l > h$ we have that $\pm g_k$ are odd while $\pm g_l \pm g_h$ are even. One can check that the one-step generator sequence starts with the first odd numbers. Let us then assume that $g_k = 2k - 1$ for all $1 \leq k \leq d$. It cannot be $g_{d+1} = 2d$ because otherwise $g_{d+1} = g_1 + g_d$. ■

The sample size increases linearly in the dimension. The sequence is not suitable for the identification of the whole parameter vector. Similar results for $F(d; m, \dots, m; 2)$, $m \geq 2$, follow later.

Theorem 50 *A Fibonacci type generator for the estimation of the main effects of the model $F(d; 1, \dots, 1; 2)$ is defined by the sequence*

$$\begin{aligned} g_1 &= 1 \\ g_2 &= 3 \\ g_d &= 2g_{d-1} + g_{d-2} + 1 \end{aligned}$$

with a size N given by the Generalised Upper Law for Main Effects.

Proof. By the formula for non-homogeneous linear recursions in Section 6.1 we have $g_d = \frac{1}{4}((1 + \sqrt{2})^{d+1} + (1 - \sqrt{2})^{d+1} - 2)$. Notice that this gives an approximated size $2g_d + g_{d-1} + 1 \approx (1 + \sqrt{2})^{d+1}$ by the Generalised Upper Law for Main Effects. It also follows that

$$\begin{aligned} 4g_d &= (1 + \sqrt{2})^{d+1} + (1 - \sqrt{2})^{d+1} - 2 \\ &= \sum_{p=0}^{d+1} \binom{d+1}{p} \sqrt{2}^p + \sum_{p=0}^{d+1} \binom{d+1}{p} (-\sqrt{2})^p - 2 \\ &= \sum_{\substack{p=0 \\ p \text{ even}}}^{d+1} \binom{d+1}{p} 2^{\frac{p}{2}} - 2. \end{aligned} \tag{6.5}$$

We have to prove the following inequalities for all i, j, l

$$g_i \neq g_j \tag{6.6}$$

$$g_i - g_j \neq g_l \tag{6.7}$$

$$g_i - g_j \neq -g_l \tag{6.8}$$

$$g_i + g_j \neq g_l \tag{6.9}$$

Inequality (6.6) holds because g_d is an increasing sequence and (6.8) is equivalent to (6.9). Let us prove (6.8). Multiplying by 4 it becomes $4g_i - 4g_j \neq 4g_l$ and substituting (6.5) it becomes

$$\sum_{\substack{p=0 \\ p \text{ even}}}^{i+1} \binom{i+1}{p} 2^{\frac{p}{2}} - 2 - \sum_{\substack{p=0 \\ p \text{ even}}}^{j+1} \binom{j+1}{p} 2^{\frac{p}{2}} - 2 \neq \sum_{\substack{p=0 \\ p \text{ even}}}^{l+1} \binom{l+1}{p} 2^{\frac{p}{2}} - 2.$$

That is

$$\sum_{\substack{p=0 \\ p \text{ even}}}^{i+1} \binom{i+1}{p} 2^{\frac{p}{2}} - \sum_{\substack{p=0 \\ p \text{ even}}}^{j+1} \binom{j+1}{p} 2^{\frac{p}{2}} - \sum_{\substack{p=0 \\ p \text{ even}}}^{l+1} \binom{l+1}{p} 2^{\frac{p}{2}} \neq -2.$$

This last inequality clearly holds since the left hand side is odd and the right hand side is even. Analogously one proves inequalities (6.9). ■

Finally, the one-step sequence of generator components for the estimation of the whole parameter vector begins with

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

and the corresponding sizes

$$*, 9, 23, 53, 97, 147, 221, 315, 425, 567, \dots$$

obtained by the Upper Law. See Table 6.3.

6.4.2 The models $F(d; 2, \dots, 2; 2)$

The array to be checked is

$$\begin{aligned} &0, \\ &\pm g_k, \pm 2g_k \qquad \qquad \qquad k = 1, \dots, d \\ &\pm g_k \pm g_\ell, \pm 2g_k \pm g_\ell, \pm 2g_k \pm 2g_\ell, \quad 1 \leq k < \ell \leq d. \end{aligned}$$

The largest number is $N_1 = 2g_d + 2g_{d-1}$ and the largest number of the first two lines is $N_3 = 2g_d$, thus the Generalised Upper Law for Main Effects gives the sample size $4g_d + 2g_{d-1} + 1$ and the Upper Law gives $4g_d + 4g_{d-1} + 1$.

Theorem 51 *The minimum power generator is given by*

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

By the Generalised Upper Law for Main Effects we get a size $4g_d + 2g_{d-1} + 1 = 22 \cdot 5^{d-2} + 1$ and for the inference on the whole parameter vector the sample size is $4g_d + 4g_{d-1} + 1 = 24 \cdot 5^{d-2} + 1$ which increases exponentially in the dimension.

Proof. It holds that $g_k \neq g_h$, $g_k \neq 2g_h$ and $2g_k \neq 2g_h$ for all k, h . For inference on the main parameters we have to prove the following inequalities for all $1 \leq k, l, m \leq d$

$$\pm g_k \neq \pm g_l \pm g_m \quad (6.10)$$

$$\pm g_k \neq \pm g_l \pm 2g_m \quad (6.11)$$

$$\pm g_k \neq \pm 2g_l \pm 2g_m \quad (6.12)$$

$$\pm 2g_k \neq \pm 2g_l \pm 2g_m \quad (6.13)$$

Inequality (6.13) is equivalent to (6.10). Inequality (6.10) is $\pm 5^k \neq \pm 5^l \pm 5^m$. We divide by $5^{\min\{k,l,m\}}$ and get $\pm 1 \neq \pm 5^p \pm 5^q$. Now

$$\pm 1 \equiv \begin{cases} 1 \pmod{5} \\ \text{or} \\ 4 \pmod{5} \end{cases}$$

while $\pm 5^p \pm 5^q \equiv 0 \pmod{5}$ for $p, q \neq 0$. The cases $p = 0$ or $q = 0$ are evident.

Inequality (6.11) is $\pm 5^k \neq \pm 2 \cdot 5^l \pm 5^m$. Dividing by $5^{\min\{k,l,m\}}$ we have two cases

$$\begin{cases} \pm 1 \neq \pm 2 \cdot 5^p \pm 5^q \\ \text{or} \\ \pm 5^p \neq \pm 2 \pm 5^q. \end{cases}$$

The first case is verified since $\pm 2 \cdot 5^p \pm 5^q \equiv 0 \pmod{5}$ which is different from $\pm 1 \pmod{5}$. We rewrite the second case as $\pm 5^p \pm 5^q \neq \pm 2$ and we conclude since $\pm 5^p \pm 5^q \equiv 0 \pmod{5}$ and $\pm 2 \equiv 2$ or $3 \pmod{5}$. Again the cases $p = 0$ or $q = 0$ are evident.

Inequality (6.12) becomes $\pm 5^k \neq 2[\pm 5^l \pm 5^m]$, which can be seen to hold by the decomposition into prime factor of the left and the right hand side.

For the inference on all the effects we have to check also the following inequalities for all $1 \leq k < h \leq d$ and $1 \leq l < m \leq d$ and not $k = l$ and $m = h$

$$\pm g_k \pm g_h \neq \pm g_l \pm g_m \quad (6.14)$$

$$\pm 2g_k \pm g_h \neq \pm g_l \pm g_m \quad (6.15)$$

$$\pm 2g_k \pm 2g_h \neq \pm g_l \pm g_m \quad (6.16)$$

$$\pm 2g_k \pm 2g_h \neq \pm 2g_l \pm g_m \quad (6.17)$$

$$\pm 2g_k \pm 2g_h \neq \pm 2g_l \pm 2g_m \quad (6.18)$$

Inequalities (6.14) and (6.18) are equivalent. Let us prove (6.14). It is $\pm 5^k \pm 5^h \neq 5^l \pm 5^m$. We divide by $\min\{k, l\}$ and get $\pm 5^p \pm 5^q \neq \pm 5^r \pm 1$. The first member is equivalent to $0 \pmod{5}$ and the second one to 1 or 4. If $k = l$ then h must be different from m and thus inequality (6.14) holds.

Inequality (6.15) is proved as follows

$$\begin{aligned} & \pm 2 \cdot 5^k \pm 5^h \neq \pm 5^l \pm 5^m \\ & \text{is equivalent to} \\ & \begin{cases} \pm 2 \cdot \pm 5^p \neq \pm 5^q \pm 5^r \\ \text{or} \\ \pm 2 \cdot 5^r \pm 5^p \neq \pm 5^q \pm 1 \end{cases} \end{aligned}$$

and again operating (mod 5) we get the assert.

With regard to inequalities (6.16) and (6.17) we have that the first member of both is divisible by 2 while the second ones are not. ■

Theorem 52 *To estimate the main effects an iterative sequence of generator components is given by*

$$\begin{aligned} g_1 &= 1 \\ g_2 &= 5 \\ g_d &= 2g_{d-1} + 2g_{d-2} + 1, \quad d \geq 3. \end{aligned}$$

Proof. We have to prove the following inequalities in \mathbb{Z} for all $1 \leq k, l, m \leq d$, $k \neq l, m$ and $l \neq m$

$$\pm g_k \neq 2g_k \quad (6.19)$$

$$\pm g_k \neq \pm g_l \pm g_m \quad (6.20)$$

$$\pm g_k \neq \pm 2g_l \pm g_m \quad (6.21)$$

$$\pm g_k \neq \pm 2g_l \pm 2g_m \quad (6.22)$$

$$\pm 2g_k \neq \pm 2g_l \pm 2g_m \quad (6.23)$$

Since g_k is odd for all k , inequalities (6.19), (6.20) and (6.22) are satisfied. Disinequality (6.23) is equivalent to inequality (6.20) and thus it holds. Let us check inequality (6.22) and rewrite it as $\pm 2g_l \neq \pm g_k \pm g_m$. The left hand side is divisible by 2 but not by 4 while the right hand side is divisible by 4. ■

From Theorem 39 we have $g_d = \frac{2}{3}((1 + \sqrt{3})^d + (1 - \sqrt{3})^d - \frac{1}{2})$ and the size given by the Generalised Upper Law for Main Effects equals approximately $(4 + \frac{8}{\sqrt{3}})(1 + \sqrt{3})^{d-1}$ and increases exponentially in the dimension.

The one-step iterative sequence of generator components for identification of main effects given by the algorithm in Table 6.2 starts as follows,

$$(1, 5, 13, 17, 37, 41, 49, 53, 109, 113, 121, 125, 145, 149, 157, 161, 325, 329\dots).$$

After inspection this sequence was found to be compatible with the following generating sequence.

Theorem 53 *The following sequence with a sample size defined by the Generalised Upper Law for Main Effects gives a lattice design suitable to identify the main effects of the model $F(d; 2, \dots, 2; 2)$*

$$\begin{aligned} g_1 &= 1 \\ g_d &= g_{d-1} + 4\alpha_{d-1} \quad d \geq 2 \\ \alpha_1 &= 1 \\ \alpha_{2^j} &= 3\alpha_{2^{j-1}} - 1 \quad j \geq 2 \\ \alpha_k &= \alpha_{2^j} \quad \text{for } k = 2^j q, \quad q \text{ odd.} \end{aligned}$$

Proof. Inequalities (6.19), (6.20) and (6.22) hold because the right hand side is even and the left hand side is odd. Inequality (6.23) is equivalent to (6.20). Let us

prove (6.21). By an easy induction step one proves that $g_k - 1$ is divisible by 4 for all k . Then (6.21) is

$$\begin{aligned} \pm g_{k-1} \pm 4\alpha_{k-1} &\neq \pm 2g_{l-1} \pm 8\alpha_{l-1} \pm g_{m-1} \pm 4\alpha_{m-1} \\ \pm g_{k-1} \mp 2g_{l-1} \mp g_{m-1} &\neq 4(\pm 2\alpha_{l-1} \pm \alpha_{m-1} \mp \alpha_{k-1}) \end{aligned}$$

The left hand side of this last inequality is not divisible by 4. ■

The difference sequence $\alpha_k, k = 1, 2, \dots$ gives

$$\begin{aligned} &1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 41, \\ &1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 122, \\ &1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 41, \\ &1, 2, 1, 5, 1, 2, 1, 14, 1, 2, 1, 5, 1, 2, 1, 365, \dots \end{aligned}$$

which shows a nice *self similar (fractal)* structure. 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 implies that g_d increases like d^γ where $\gamma = \frac{\log 3}{\log 2} \approx 1.5850$, a number which is reminiscent of results in fractal dimension. Hence we can take sizes N which increase like d^γ as the dimension d increases.

Theorem 54 *The following iterative sequence of generator components*

$$\begin{aligned} g_1 &= 1 \\ g_2 &= 5 \\ g_d &= 4g_{d-1} + 2g_{d-2} + 1, \quad d \geq 3 \end{aligned}$$

with a size given by the Upper Law generates a design orthogonal for the model $F(d; 2, \dots, 2; 2)$.

By Theorem 39 we have that

$$g_d = \frac{1}{30} \left((3 + 2\sqrt{6})(2 + \sqrt{6})^d + (3 - 2\sqrt{6})(2 - \sqrt{6})^d - 6 \right)$$

and the support size is approximately equal to $\frac{1}{5}(4 + \sqrt{6})(2 + \sqrt{6})^d$ by the *Upper Law*.

The one-step sequence of generator components

$$(1, 5, 23, 60, 77, 173, 222, 409, 535, 634, 935, 1182, 1361, 1497, \dots) \tag{6.24}$$

and the corresponding sizes

$$*, 25, 113, 333, 549, 1001, 1581, 2525, 3777, 4677, 6277, 8469, 10173, 11533, \dots$$

obtained by the Upper Law. See Table 6.3.

6.4.3 The models $F(d; m, \dots, m; 2)$

The array to be checked becomes

$$\begin{array}{l} 0 \\ \pm g_k \quad \pm 2g_k, \dots, \pm mg_k \quad k = 1, \dots, d \\ \pm ag_k \pm bg_l \quad 1 \leq k < l \leq d \quad \text{and} \quad 1 \leq a, b \leq m. \end{array} \tag{6.25}$$

The largest element in the array is $N_1 = m(g_d + g_{d-1})$ and the largest element in the first two rows is $N_3 = mg_d$.

Theorem 55 *The minimum power generator has base $2m + 1$ for inference both on the main effects and the whole parameter vector. The sample size given by the Generalised Upper Law for main effects is $N_M = m(4m + 3)(2m + 1)^{d-2} + 1$ and by the Upper Law we have $N = 4m(m + 1)(2m + 1)^{d-2} + 1$.*

Proof. Clearly any smaller base is not suitable. For the inference on the whole parameter vector we have to prove that the positive entries in Array (6.25) are distinct in \mathbb{Z} . Indeed we have $ag_k < bg_l$ for all $1 \leq k < l \leq d$ and for all $a, b \in \{1, \dots, m\}$ since $a(2m + 1)^{k-1} < b(2m + 1)^{l-1}$ is implied by $a < b(2m + 1)^{l-k}$ which clearly holds.

Inequality $bg_l \pm ag_k \neq cg_l$ for all $1 \leq k < l \leq d$ and for all $a, b, c \in \{1, \dots, m\}$ and for all $1 \leq j \leq d$ is

$$b(2m + 1)^{l-1} \pm a(2m + 1)^{k-1} \neq c(2m + 1)^{j-1}.$$

For $l < j$ we divide by the common factor $(2m + 1)^{l-1}$ and get $b \pm a(2m + 1)^{k-l} \neq c(2m + 1)^{j-l}$. Passing (mod $2m + 1$) we have $b \neq 0$ which holds. Analogously one treats the case $j < l$ dividing by $(2m + 1)^{j-1}$ while the case $j = l$ clearly holds.

Inequality $bg_l \pm ag_k \neq cg_j \pm dg_s$ for all $1 \leq k < l \leq d$ and $1 \leq s < j \leq d$ and all $a, b, c, d \in \{1, \dots, m\}$ becomes

$$b(2m + 1)^{l-1} \pm a(2m + 1)^{k-1} \neq c(2m + 1)^{j-1} \pm d(2m + 1)^{s-1}.$$

For $k \leq s$ we divide by $(2m + 1)^{k-1}$ and have

$$a \pm b(2m + 1)^{l-k} \neq c(2m + 1)^{j-k} \pm d(2m + 1)^{s-k}.$$

We work (mod $2m + 1$). For $s \neq k$ we have $a \pmod{2m + 1} \neq 0$ which holds. For $s = k$ and $a \neq c$ we have $a \pmod{2m + 1} \neq c \pmod{2m + 1}$ which holds. The case $s = k$ and $a = c$ has already been treated.

For inference of the main effects only we work (mod N_M). As above we have $\pm ag_k \neq \pm bg_l \pmod{N_M}$ for all $a, b \in \{1, \dots, m\}$ and $1 \leq k < l \leq d$ and also

$$ag_l \pm bg_k \neq \pm cg_j$$

for all $1 \leq k < l \leq d, q \leq j \leq d$ and $a, b, c, \in \{1, \dots, m\}$.

With regard to the negative entries we have that

$$(-ag_l \pm bg_k) \pmod{N_M} \neq cg_j \pmod{N_M}$$

that is

$$m(4m + 3)(2m + 1)^{d-2} + 1 - a(2m + 1)^{l-1} \pm b(2m + 1)^{k-1} \neq c(2m + 1)^{j-1}$$

and that the left hand side is

$$\begin{cases} 1 \pmod{2m + 1} & \text{for } k \neq 1 \\ 1 \pm b \pmod{2m + 1} & \text{for } k = 1 \end{cases}$$

and the right hand side is

$$\begin{cases} 0 \pmod{2m + 1} & \text{for } j \neq 1 \\ c \pmod{2m + 1} & \text{for } j = 1 \end{cases}$$

After a little more work one sees that they are different. ■

The following theorems are proved in analogy to the theorems of Section 6.4.3 reasoning (mod m) instead of (mod 2).

Theorem 56 *The following sequence generates a lattice design for inference on main effects of the model $F(d; m, \dots, m; 2)$*

$$\begin{aligned} g_1 &= 1 \\ g_2 &= 2m + 1 \\ g_d &= m(g_{d-1} + g_{d-2}) + 1, \quad d \geq 3 \end{aligned}$$

By the linear non-homogeneous recursion formula we obtain the solution

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

and by the Generalised Upper Law for Main Effects the support size is

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

which increases exponentially in the dimension.

In generalisation of the case $m = 2$ we obtain the following iterative sequence of generator components which is increasing at most polynomially in the dimension

$$\begin{aligned} g_1 &= 1, \\ g_d &= g_{d-1} + 2m\alpha_{d-1}, \quad d \geq 2; \\ \alpha_1 &= 1, \\ \alpha_{2j} &= (m+1)\alpha_{2j-1} - 1, \quad j \geq 2 \\ \alpha_k &= \alpha_{2j}, \quad \text{for } k = 2^j q, \quad q \text{ odd.} \end{aligned}$$

The difference sequence again shows a *self similar* structure. After some algebra we obtain $\alpha_{2j} = \frac{(m-1)(m+1)^j + 1}{m}$ and $g_{2j} = 2m(m+1)^j + 1$. This implies that g_d increases like d^γ where $\gamma = \frac{\log(m+1)}{\log 2}$.

Turning to inference on the whole parameter vector we have the following theorem.

Theorem 57 *An iterative sequence of generator components for inference on the whole parameter vector of the model $F(d; m, \dots, m; 2)$ is*

$$\begin{aligned} g_1 &= 1, \\ g_2 &= 2m + 1, \\ g_d &= m(2g_{d-1} + g_{d-2}) + 1, \quad d \geq 3 \end{aligned}$$

with a sample size given by the Upper Law.

By Theorem 39 we have

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

and the approximated size

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

As for the additive models we summarise the results in self-explanatory tables.

We conclude our presentation with some figures representing the behaviour 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 $F(d; 2, \dots, 2; 2)$ Figure 1 shows the logarithm of α_d , the first differences of the generators divided by 4, over the dimension d for the sequence in Theorem 53 up to $d = 180$. The self similar structure mentioned above 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 $F(d; 2, \dots, 2; 2)$ Figure 3 shows the logarithm $\log(g_d)$ of the generators for the one-step sequence (6.24) 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 the dimension d with γ approximately equal to the estimated slopes. Note that the estimate 1.7 for the analysis of the main effects slightly over-estimates $\gamma = \frac{\log 3}{\log 2} \approx 1.5850$.

Summary

In this chapter we tackle the so-called inverse problem. That is, given a class of Fourier models indexed over the dimension we look for one-generator lattice designs which are orthogonal for the models in the class as an alternative to product designs which require a much larger sample size. In particular lattice designs with a sample size of the order of the number of parameters in the models are found for certain classes of models. Various methods are described and in particular an algorithm is given such that the sample size of the resulting orthogonal design increases polynomially in the dimension.

Special attention is given to additive and two-factor interaction models since for these classes of models the difference between the number of parameters and the sample size of product designs is largest.

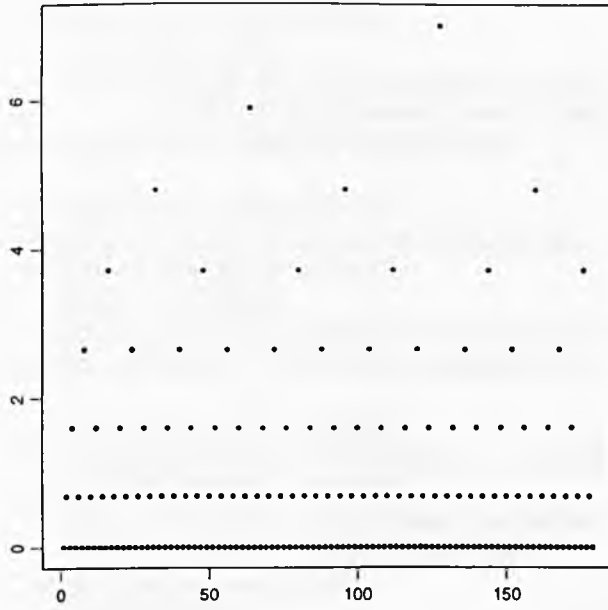


Figure 6.1: Main effect of the model $F(d; 2, \dots, 2; 2)$: $\log(\alpha_d)$ over d .

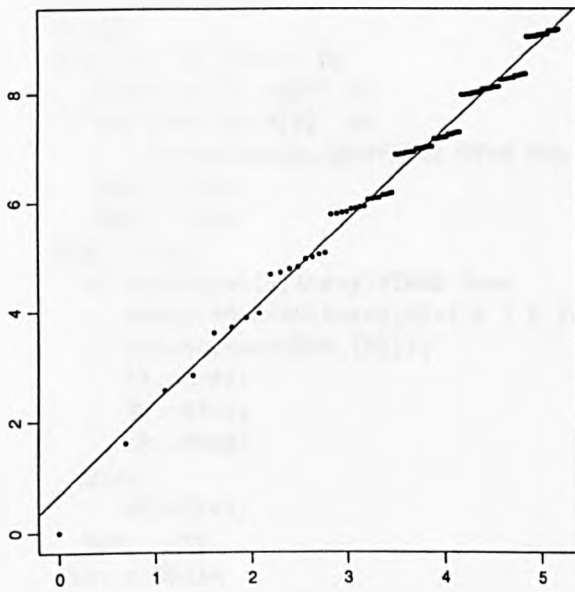


Figure 6.2: Main effects of the model $F(d; 2, \dots, 2; 2)$: $\log(g_d)$ over $\log(d)$.

```

/*****
  InterList check in two lists do not have common elements
  *****/
-- Input: two list
-- Output: FALSE if the intersection is not empty
--         TRUE if the intersection is empty
InterList(A,V):= EqSet(Diff(A,V),A);

/*****
  AbsVal returns the absolute value of the input number
  *****/
-- Input: a numberN
-- Output: N if N is positive and -N if N is negative
Define AbsVal(N) If N>0 Then Return(N) Else Return(-N) End; End;

/*****
  One-step generator for  $F(d;m_1,\dots,m_d;2)$  main effects
  *****/
-- Input: The vector containing the orders of the marginal models
-- Output: the list of generators Gen
Define OneStepTwoMain(M)
  Dimen:=Len(M);
  Gen:=[1];
  Array:=[ K | K In 1..M[1] ];
  DT:=2;
  TAG:=TRUE;
  GT:=M[1]+1;
  While (DT<=Dimen) Do
    OK:=FALSE;
    While OK=FALSE Do
      B:=[];
      For J:=1 To (DT-1) Do
        For K:=1 To M[DT] Do
          For H:=1 To M[J] Do
            B:=Concat(B,[AbsVal(K GT+H Gen[J])],[AbsVal(K GT-H Gen[J])]);
          End; --For
        End; --For
      End; --For
      If InterList(B,Array)=TRUE Then
        Array:=Concat(Array,GT+[ K | K In 1..M[DT] ]);
        Gen:=Concat(Gen,[GT]);
        DT:=DT+1;
        GT:=GT+1;
        OK:=TRUE;
      Else
        GT:=GT+1;
      End; --If
    End; --While
  End; --While
  Return(Gen);
End;

```

Table 6.2: Code for the one-step strategy for the main effects of $F(d; m_1, \dots, m_d; 2)$.

```

/*****
One-step generator for  $F(d; m_1, \dots, m_d; 2)$ 
*****/
-- Input: The vector containing the orders of the marginal models
-- Output: the list of generators
Define OneStepTwoAll(M)
  Dimen:=Len(M); Gen:=[1]; Array:=[ K | K In 1..M[1] ];
  DT:=2; TAG:=TRUE; GT:=M[1]+1;
  While (DT<=Dimen) Do
    If TAG=TRUE Then
      S:=Max(Array);
      C:=[ K | K In 1..S];
      Candidates:=Diff(C,Array);
      If Candidates<>[] Then
        GT:=First(Candidates); Candidates:=Diff(Candidates,[GT]);
      Else GT:=S+1;
      End; --If
    End; --If
    B:=[];
    For K:=1 To M[DT] Do
      B:=Set( Concat(B,[K AbsVal(GT)]) )
    End; -- For
    For J:=1 To (DT-1) Do
      For K:=1 To M[DT] Do
        For H:=1 To M[J] Do
          B:=Sorted( Set( Concat(B,[AbsVal(K GT+H Gen[J])],
                                [AbsVal(K GT-H Gen[J])]) ) );
        End; --For
      End; --For
    End; --For
    If InterList(Array,B)=TRUE Then
      Array:=Sorted( Set( Concat(B,Array) ) );
      Gen:=Concat(Gen,[GT]); DT:=DT+1; TAG:=TRUE;
    Else
      TAG:=FALSE;
      If Candidates<>[] Then
        GT:=First(Candidates); Candidates:=Diff(Candidates,[GT]);
      Else GT:=GT+1;
      End; --If
    End; --If
  End; --While
  Return(Gen);
End;

```

Table 6.3: Code for the one-step strategy for all the effects of $F(d; m_1, \dots, m_d; 2)$.

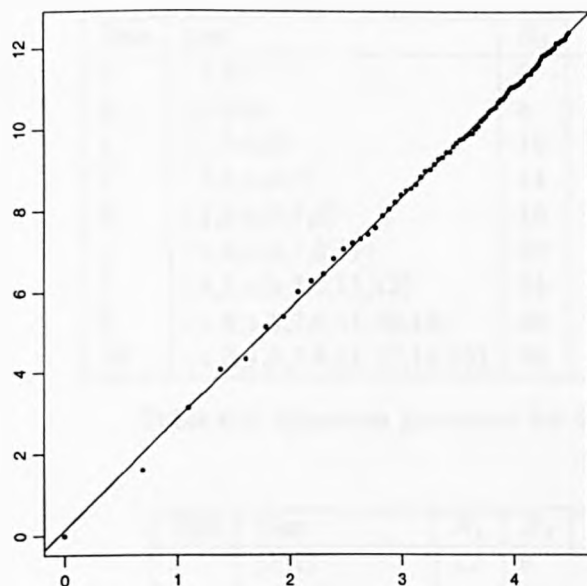


Figure 6.3: All effects of the model $F(d; 2, \dots, 2; 2)$; $\log(g_d)$ over $\log(d)$.

Dim	gen	N_1	N_2	UL	Gen UL	Min.Size
2	(1,3)	6	3	13	10	10
3	(1,3,5)	10	6	21	17	14
4	(1,3,5,7)	14	10	29	25	18
5	(1,3,5,7,9)	18	14	37	33	22
d	$(1, 3, \dots, 2d - 1)$	$4d - 2$	$4d - 6$	$8d - 3$	$8d - 7$	$4d + 2$

Table 6.4: Linear type generator for the models $F(d; 2, \dots, 2; 1)$.

Dim	gen	N_1	N_2	UL	Gen UL	Min.Size
2	(1,4)	12	8	25	21	17
3	(1,4,7)	21	14	43	36	27
4	(1,4,7,10)	30	21	61	52	36
5	(1,4,7,10,13)	39	30	79	70	45
d	$g_d = 3d - 2$	$9d - 6$	$9d - 15$	$18d - 11$	$18d - 20$	$9d$

Table 6.5: Linear generator for the models $F(d; 3, \dots, 3; 1)$.

Dim	gen	N_1	N_2	UL	Gen UL	Min.size
2	(1,5)	20	15	41	36	26
3	(1,5,9)	36	27	73	64	43
4	(1,5,9,13)	52	39	105	92	58
5	(1,5,9,13,17)	68	52	137	121	74
d	$g_d = 4d - 3$	$16d - 12$	$16d - 28$	$32d - 23$	$32d - 39$	$16d - 6$

Table 6.6: Linear generator for the models $F(d; 4, \dots, 4; 1)$.

Dim	gen	N_1	N_2	UL	Gen UL	Min.size
2	(1,3)	6	3	13	10	10
3	(1,3,4)	8	6	17	15	13
4	(1,3,4,5)	10	8	21	19	17
5	(1,3,4,5,7)	14	10	29	25	23
6	(1,3,4,5,7,9)	18	14	37	33	29
7	(1,3,4,5,7,9,11)	22	18	45	41	34
8	(1,3,4,5,7,9,11,12)	24	22	49	47	37
9	(1,3,4,5,7,9,11,12,13)	26	24	53	51	41
10	(1,3,4,5,7,9,11,12,13,15)	30	26	61	57	46

Table 6.7: One-step generator for the models $F(d; 2, \dots, 2; 1)$.

Dim	Gen	N_1	N_2	UL	Gen UL	Min.size
2	(1,4)	12	8	25	21	17
3	(1,4,5)	15	12	31	28	21
4	(1,4,5,7)	21	15	43	37	32
5	(1,4,5,7,9)	27	21	55	49	38
6	(1,4,5,7,9,11)	33	27	67	61	46

Table 6.8: One-step generator for the models $F(d; 3, \dots, 3; 1)$.

Dim	gen	N_1	N_2	UL	Gen UL	Min.size
2	(1,5)	20	15	41	36	26
3	(1,5,6)	24	20	49	45	31
4	(1,5,6,7)	28	24	57	53	37
5	(1,5,6,7,11)	44	33	89	78	60
6	(1,5,6,7,11,13)	52	44	105	97	69

Table 6.9: One-step generator for the models $F(d; 4, \dots, 4; 1)$.

$F(d; 1, \dots, 1; 2)$	$N_1 = g_d + g_{d-1}$	$N_3 = g_d$
MAIN EFFECTS		Main gen UL
Min power gen	$g_d = 3^{d-1}$	$7 \cdot 3^{d-2} + 1$
Fibonacci type	$g_d = 2^d - 1$	$5 \cdot 2^{d-1} + 2$
One-step	$g_d = 2d - 1$	$6d - 4$
ALL EFFECTS		UL
Min power gen	$g_d = 3^{d-1}$	$8 \cdot 3^{d-2} + 1$
Fibonacci type	$\begin{cases} g_1 = 1 \\ g_2 = 3 \\ g_d = 2g_{d-1} + g_{d-2} + 1 \end{cases}$	$\approx \frac{1}{\sqrt{2}}(1 + \sqrt{2})^{d+1}$
One-step	(1, 3, 8, 18, 30, 43, ...)	(* , 9, 23, 53, 97, 147, ...)

Table 6.10: Models with two-factor interaction and first order marginal.

$F(d; 2, \dots, 2; 2)$	$N_1 = 2(g_d + g_{d-1})$	$N_3 = 2g_d$
MAIN EFFECTS		Main Gen UL
Min power gen	$g_d = 5^{d-1}$	$22 \cdot 5^{d-2} + 1$
Fibonacci type	$\begin{cases} g_1 = 1 \\ g_2 = 5 \\ g_d = 2g_{d-1} + 2g_{d-2} + 1 \end{cases}$	$\approx 2(1 + \sqrt{3})^{d+1}$
One-step	$\begin{cases} g_1 = 1 \\ g_d = g_{d-1} + 4\alpha_{d-1} \\ \alpha_1 = 1 \\ \alpha_{2j} = 3\alpha_{2j-1} - 1 \text{ for } j \geq 2 \\ \alpha_k = \alpha_{2j} \text{ for } k = 2^j q, q \text{ odd} \end{cases}$	growth: d^γ with $\gamma = \frac{\log 3}{\log 2}$
ALL EFFECTS		UL
Min power gen	$g_d = 5^{d-1}$	$24 \cdot 5^{d-2} + 1$
Fibonacci type	$\begin{cases} g_1 = 1 \\ g_2 = 5 \\ g_d = 4g_{d-1} + 2g_{d-2} + 1 \end{cases}$	$\approx 2(2 + \sqrt{6})^d$
One-step	(1, 5, 23, 60, 77, ...)	(* , 25, 113, 333, 549, ...)

Table 6.11: Models with two-factor interaction and second order marginal.

$F(d; m, \dots, m; 2)$	$N_1 = m(g_d + g_{d-1})$	$N_3 = mg_d$
MAIN EFFECTS		Main Gen UL
Min power gen	$g_d = (2m + 1)^{d-1}$	$m(4m + 3)(2m + 1)^{d-2} + 1$
Fibonacci type	$\begin{cases} g_1 = 1 \\ g_2 = 2m + 1 \\ g_d = m(g_{d-1} + g_{d-2}) + 1 \end{cases}$	$\approx c(m)^\dagger \left(\frac{m + \sqrt{m^2 + 4m}}{2} \right)^{d-1}$
“One-step” (self-similar)	$\begin{cases} g_1 = 1 \\ g_d = g_{d-1} + 2m\alpha_{d-1} \\ \alpha_1 = 1 \\ \alpha_{2j} = (m + 1)\alpha_{2j-1} - 1 \text{ for } j \geq 2 \\ \alpha_k = \alpha_{2j} \text{ for } k = 2^j q, q \text{ odd} \end{cases}$	growth: d^γ with $\gamma = \frac{\log(m+1)}{\log 2}$
ALL EFFECTS		UL
Min power gen	$g_d = (2m + 1)^{d-1}$	$4m(m + 1)(2m + 1)^{d-2} + 1$
Fibonacci type	$\begin{cases} g_1 = 1 \\ g_2 = 2m + 1 \\ g_d = m(2g_{d-1} + g_{d-2}) + 1 \end{cases}$	$\approx c'(m)^\ddagger \left(m + \sqrt{m(m + 1)} \right)^d$

$\dagger c(m) = \frac{m^2}{2m-1} \left(3 + \frac{5m+2}{\sqrt{m^2+4m}} \right)$ and $\lim_{m \rightarrow \infty} c(m) = +\infty$; $\ddagger \lim_{m \rightarrow \infty} c'(m) = 1$

Table 6.12: Models with two-factor interaction and equal order marginal.

Chapter 7

Lattice designs for screening experiments

Integer lattices can be used to fit models, or *emulators*, to complex functions. Examples include high dimensional functions and the computer output from programmes arising from CAE (Computer Aided Engineering) or other modelling situations. Fourier models are fitted using the discrete and fast Fourier Transform and the power spectrum is used to detect important factors.

Complex systems can be very expensive to model, either because of their high dimensionality or a heavy computational or experimental cost. Nowadays a common strategy is to model a complex system with an emulator performing experiments on the system directly. In the statistical literature this has been referred to as DACE: the Design and Analysis of Computer Experiments, see Sacks, Welch, Mitchell and Wynn (1989) [62]. In the engineering and CAE literature it is referred to as the method of surrogates, see Yeşilyurt and A. T. Patera (1995) [76].

We wish to investigate the input variables or process parameters, which and to what order, can be identified to build an emulator consisting of a submodel of some larger Fourier model. In practice we will be looking for an additive Fourier model that approximates a supermodel and that involves less factors than the supermodel.

To identify these parameters of interest (including higher order terms) we work in a one-dimensional frequency domain using the lattice structure and apply the Fourier Transform (FT, [73]). We use the macros for the calculation of the fast FT and of the spectrum included in the statistical package Splus. We then return to the original parameters using the inverse of the mapping into the one-dimensional frequency domain.

We clarify the use of the FT tool with simple examples. Suppose we want to fit the additive model $F(2; 1, 1; 1)$ to a real process evaluated at design points which form an orthogonal set for the complete model $F(2; 1, 1; 2)$. We write the full model in complex form

$$\begin{aligned} E(Y(x_1, x_2)) = d_0 &+ \sqrt{2}d_1e^{i2\pi x_1} + \sqrt{2}d_{-1}e^{-i2\pi x_1} \\ &+ \sqrt{2}d_2e^{i2\pi x_2} + \sqrt{2}d_{-2}e^{-i2\pi x_2} \\ &+ \sqrt{2}d_3e^{i2\pi(x_1+x_2)} + \sqrt{2}d_{-3}e^{-i2\pi(x_1+x_2)} \\ &+ \sqrt{2}d_4e^{i2\pi(x_1-x_2)} + \sqrt{2}d_{-4}e^{-i2\pi(x_1-x_2)}. \end{aligned}$$

Consider the design generated by (1, 5) with 13 points, which is orthogonal for

inference on the main coefficients ($d_{-2}, d_{-1}, d_0, d_1, d_2$). Figure 7.1 shows the following 13 observations made at the lattice design points

$$Y_i : 1 \ 2 \ 3 \ 4 \ 4 \ 1 \ 1 \ 1 \ 2 \ 3 \ 3 \ 3 \ 2$$

Applying standard Fourier transform methods we may compute the coefficients, c_i , of the orthogonal trigonometric representation (Fourier series) of the $Y_t, t = 0, \dots, 12$

$$\begin{aligned} Y_t = c_0 &+ c_1 e^{i\frac{2\pi}{13}t} + c_{-1} e^{-i\frac{2\pi}{13}t} \\ &+ c_2 e^{i\frac{2\pi}{13}2t} + c_{-2} e^{-i\frac{2\pi}{13}2t} \\ &+ c_3 e^{i\frac{2\pi}{13}(3)t} + c_{-3} e^{-i\frac{2\pi}{13}3t} \\ &+ c_4 e^{i\frac{2\pi}{13}(4)t} + c_{-4} e^{-i\frac{2\pi}{13}4t} \\ &+ c_5 e^{i\frac{2\pi}{13}(5)t} + c_{-5} e^{-i\frac{2\pi}{13}5t} \\ &+ c_6 e^{i\frac{2\pi}{13}(6)t} + c_{-6} e^{-i\frac{2\pi}{13}6t}. \end{aligned} \quad (7.1)$$

We recall the following well-known facts from Fourier and Spectral Analysis. The power of a finite sequence Y_t ($t = 0, \dots, N - 1$) is defined as

$$\sum_{t=0}^{N-1} Y_t^2 = N \sum_{t=0}^{N-1} |c_t|^2.$$

When the Fourier series of the observed values is written in real form, let θ_t and ϕ_t represent the coefficients of the cosine and sine terms of the t -th frequency respectively. Then the value of the power spectrum f_t at the t -frequency is defined as

$$\begin{cases} f_0 = |c_0|^2 = \theta_0^2 \\ f_t = 2|c_t|^2 = \frac{1}{2}(\theta_t^2 + \phi_t^2) \quad \text{for } t = 1, \dots, \left[\frac{N}{2}\right]. \end{cases}$$

Hence the plot of f_t against t describes how the total power is distributed over the various frequency components of the observed sequence. An equivalent interpretation is the regression sum of squares for the relevant term. The plots of the next sections are done using the Splus function spectrum with argument pgram which estimates the spectrum *by taking the discrete Fourier transform of the (detrended then tapered then padded) data. The squared modulus of this transform is then smoothed by a sequence of running averages. See Bloomfield (1976) [10] for a discussion of the method.* (Quoted from the on line help of Splus Version 3.4, 1996). The tapering value is .1 times the length of the time series. The padded value is zero and the detrending operation removes a least square line from the time series before computing the periodogram. The mean is not removed. That is why the values f_t plotted in the next figures can be negative.

Returning to the example, we restrict the input parameters of the model $F(2; 1, 1; 2)$ to the "line" $\{(s, 5s \pmod{1}) : s \in \mathbb{R}\}$ on which the lattice points lie. Visualised on the plane $[0, 1]^2$ this line is a step function but on the torus defined by the standard isomorphism from $[0, 1]^2$ to $S_1 \times S_1$ it is a spiral. We take parametric coordinates on this spiral normalised to 13 and denote it by s . Thus for $s = [0, 13[$

the $F(2; 1, 1; 2)$ model becomes

$$\begin{aligned} E(Y(x_1(s), x_2(s))) = & d_0 + \sqrt{2}d_1e^{i\frac{2\pi}{13}s} + \sqrt{2}d_{-1}e^{-i\frac{2\pi}{13}s} \\ & + \sqrt{2}d_2e^{i\frac{2\pi}{13}5s(\text{mod } 13)} + \sqrt{2}d_{-2}e^{-i\frac{2\pi}{13}5s(\text{mod } 13)} \\ & + \sqrt{2}d_3e^{i\frac{2\pi}{13}(s+5s(\text{mod } 13))} + \sqrt{2}d_{-3}e^{-i\frac{2\pi}{13}(s+5s(\text{mod } 13))} \\ & + \sqrt{2}d_4e^{i\frac{2\pi}{13}(s-5s(\text{mod } 13))} + \sqrt{2}d_{-4}e^{-i\frac{2\pi}{13}(s-5s(\text{mod } 13))}. \end{aligned}$$

Since the following equalities hold

$$\begin{aligned} e^{i\frac{2\pi}{13}5s(\text{mod } 13)} &= e^{i\frac{2\pi}{13}5s} \\ e^{i\frac{2\pi}{13}(s+5s(\text{mod } 13))} &= e^{i\frac{2\pi}{13}6s} \\ e^{i\frac{2\pi}{13}(s-5s(\text{mod } 13))} &= e^{i\frac{2\pi}{13}9s}, \end{aligned}$$

we can write

$$\begin{aligned} E(Y(x_1(s), x_2(s))) = & d_0 + \sqrt{2}d_1e^{i\frac{2\pi}{13}s} + \sqrt{2}d_{-1}e^{-i\frac{2\pi}{13}s} \\ & + \sqrt{2}d_2e^{i\frac{2\pi}{13}5s} + \sqrt{2}d_{-2}e^{-i\frac{2\pi}{13}5s} \\ & + \sqrt{2}d_3e^{i\frac{2\pi}{13}6s} + \sqrt{2}d_{-3}e^{-i\frac{2\pi}{13}6s} \\ & + \sqrt{2}d_4e^{i\frac{2\pi}{13}9s} + \sqrt{2}d_{-4}e^{-i\frac{2\pi}{13}9s}. \end{aligned} \quad (7.2)$$

The key point is then to consider this as a one dimensional model with s as the variable. The input parameter x_1 is associated with the frequency $\omega_1 = 1$, x_2 with $\omega_5 = 5$, the interaction $x_1 + x_2$ with $\omega_6 = 6$ and $x_1 - x_2$ with $\omega_9 = 9$. Indeed compare the discrete formula (7.1) with the continuous one (7.2) by letting $t = s$ and $c_i = \sqrt{2}d_i$. The terms for the main effects are in both formulae and from the spectral analysis for the Y_i 's we are able to extract the important frequencies for (7.2). Then using the mapping $x_1 \leftrightarrow 1$ $x_2 \leftrightarrow 5$ $x_1 + x_2 \leftrightarrow 6$ we deduce which coefficients in $F(2; 1, 1; 2)$ are to be selected for investigation. Note that $x_1 - x_2 \leftrightarrow 9$ is not available because only the frequencies up to order 6 ($= \left[\frac{13}{2} \right]$) are recognised by the Fourier transform. Since we are interested in the main effects this does not prove restrictive.

From the power spectrum plot, Figure 7.2, we deduce that the most influential frequency is at $t = 2$. This is confirmed by the direct evaluation of the Fourier coefficients in (7.1)

$$\begin{aligned} c_0 &= 30.000000 + 0.000000i \\ c_1 &= 2.124319 - 1.264602i & c_2 &= -8.759016 - 0.568902i \\ c_3 &= -0.420373 + 2.222723i & c_4 &= 0.355769 - 0.767301i \\ c_5 &= -2.143804 - 1.048391i & c_6 &= 0.343106 + 1.094877i, \end{aligned}$$

and their squared norms show the key role of the second frequency

$$900.000000 \quad 6.111952 \quad \underline{77.044014} \quad 5.117213 \quad 0.715323 \quad 5.695021 \quad 1.316477.$$

The value at the frequency 0 corresponds to the mean of the observations. It was convenient to exclude this from the plot because of its typically high value.

The power spectrum shows both x_1 and x_2 (corresponding to frequency points 1 and 5 respectively) as being significant with x_1 having the larger effect. From this

we could infer the slightly greater importance of the variable x_1 . The largest point on the spectrum is however the second frequency point and we offer the following explanation. The lattice design generated by (1, 5) with 16 points is orthogonal also for the model $F(2; 2, 2; 2)$. The analysis carried for $F(2; 1, 1; 2)$ with the same generator (1, 5) but with 13 points suggests that a screening on the second order model for the first variable could be significant, due to the predominant role of the frequency corresponding to $2x_1$. This is confirmed by the plot of the power spectrum for the 16-point model comprising the 13 original points and $Y_{14} = 1, Y_{15} = 1, Y_{16} = 2$, see Figures 7.3 and 7.4. Thus a better emulator than $F(2; 1, 1; 1)$ would be $F(2; 2, 1; 1)$.

7.1 Analysis of a known function

As a second example we take observations from the function

$$Y(x_1, x_2, x_3) = x_1^{x_3}.$$

The lattice design generated by (1, 61, 11) and with a minimal sample size of 721 points is orthogonal for investigating the effects of the main parameters of the Fourier regression model $F(3; 5, 5, 5; 2)$.

Figure 7.5 shows the observed values and Figure 7.6 their power spectrum on a decibel scale. The highest peaks except the grand mean, correspond to the frequency multiple of 11, showing the large influence of the third coordinate. The sum of the power spectrum for these frequencies is -13.5 compared with -101.9 for those of the first coordinate and -146.4 for the second coordinate. Therefore the Fourier model $F(3; 5, 0, 1; 1)$ could be a suitable emulator for the above function.

Note that the given model is bidimensional being of order 0 at the second coordinate and this has been detected correctly by the analysis carried on the power spectrum plot. Figure 7.7 shows the spectrum for the frequencies higher than -15 from the previous plot and the labels indicate the corresponding frequency for each interesting line. The vertical values of the plot has been plotted as the increment above 50. A similar shift applies to other similar plots below. To aid interpretation the plot has been raised by the minimum frequency value. The actual frequency values plotted are 1, 8, 9, 10, 11, 12, 13, 14, 20, 21, 22, 23, 32, 33, 34, 44, 45, 55, 66, 77, 88, 99, 110. Notice that this sequence includes the multiples of 11 that is the third coordinate, as expected.

Since the first coordinate corresponds to the frequencies 1, 2, 3, 4, 5, its relevance might be underestimated by being condensed into the first part of the plot. In order to investigate its contribution the generator (11, 61, 1) has been considered again with sample size 721. The relevant plots are shown in Figures 7.8, 7.9 and 7.10. Again the peaks are at the frequencies multiple of 11 that now correspond to the first coordinate. The sum of the squared values of the power spectrum for these frequencies is 5.5 and for the frequencies corresponding to the third coordinate it is -93.2 . A better emulator for the given function is then represented by the model $F(3; 5, 0, 5; 1)$ which does not favour either the first coordinate or the third over the other one and recognises the relative unimportance of the variable x_2 .

Next we add a small contribution from the second input variable by considering

the function

$$Y(x_1, x_2, x_3) = x_1^{x_3+0.1x_2}$$

and maintaining the same regression model and designs. Figures 7.11 and 7.12 shows the observed values and the power spectrum for the generator (1, 61, 11) and Figures 7.14 and 7.15 show the plots for the generator (11, 61, 1). Figures 7.13 and 7.16 give the frequencies where the power spectrum exceeds -15 . Compared to observations from the previous function there is evidence of the contribution from x_2 in the plots. In the first case the sum of the frequencies significant to x_3 is -15.9 , for x_1 it is -105.4 and for x_2 it is -124.1 . In the second case we have 7.8 for x_1 , -109.3 for x_2 and -95.7 for x_3 .

As a more complicated example we consider 23 dimensions and make observations from the function

$$\begin{aligned} y = & \frac{5x_{12}}{1+x_1} + 5(x_4 - x_{20})^2 + x_5 + 40x_{19}^3 - 5x_{19} - .05x_2 \\ & + .08x_3 - .03x_7 + .01x_8 - .02x_9 - .01x_{10} - .07x_{11} + .25x_{13}^2 - .04x_{14} \\ & + .06x_{15} - .01(x_{16} + x_{17}) - .03x_{18} + .0033x_{21} - .0021x_{22} + .02x_{23} \end{aligned}$$

where $x_i \in [0, 1]$ for each $i \in \{1, \dots, 23\}$. The important variables are x_4 , x_5 , x_{12} , x_{19} and x_{20} (see Welch et al, 1992).

The observations are taken at the design points defined by the lattice with 134 points and generated by

$$g_i = 2i - 1 \quad (i = 1, \dots, 23).$$

That is the first 23 odd numbers. The generated design is orthogonal for investigating the main effects for the model $F(23; 1, \dots, 1; 2)$ where only a first order effect is considered for each variable. Thus the input factor x_1 corresponds to $g_1 = 1$, the first frequency, x_2 to $g_2 = 3$, the third frequency, x_3 to $g_3 = 5$, the fifth frequency, and so on. Figure 7.17 shows the values of y at the design points, Figure 7.18 the power spectrum in decibel scale and Figure 7.19 shows the values of the spectrum corresponding to the highest frequencies and the labels indicate to which variable (if any) that frequency corresponds. We note the predominant effect of x_5 , x_{12} , x_{19} , x_{20} as expected in Welch et al. (1992). However there is also a strong influence from other variables while the effect of x_4 has not been detected. Moreover, the presence of so many high frequencies between frequencies corresponding to variables suggests that a higher order model would be more suitable to emulate the given function.

Figure 7.20 shows the frequencies higher than 10 where the function has been evaluated at the lattice design generated by

$$g_i = 3i - 2 \quad (i = 1, \dots, 23)$$

and with sample size 207. The given design is orthogonal for the linear Fourier model of order 3, $F(d; 3, \dots, 3; 1)$. The mapping from the frequency to the corresponding variable is variable = (frequency + 2)/3, for example the label 55 corresponds to variable x_{19} . Of course after frequency 67 there is no corresponding variable. From this plot we could argue that a suitable emulator is

$$F(23; 1, 1, 2, 2, 0, 1, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0, 3, 3, 1, 1, 0, 1).$$

7.2 The fitted model

In the usual regression setup, assuming the original model is correct, we can estimate the model mean $\mu(x)$ at a particular x by the unbiased estimator

$$\hat{\mu}(x) = X(x)\hat{\theta} = Z(x)\hat{\alpha}.$$

Under the orthogonality conditions, the variance of estimation under the model A is easily seen to be

$$\text{Var}(\hat{\mu}(x)) = E(\hat{\mu}(x) - \mu(x))^2 = \frac{\sigma^2}{N} \#(A)$$

where σ^2 is the error variance. Under the Kiefer-Wolfowitz theory $\max \text{Var}(\hat{\mu}(x))$ over $[0, 1]^d$ is also minimised: G -optimality. The integrated variance is

$$I_1 = \int_{[0,1]^d} \#(A) \frac{\sigma^2}{N} dx = \#(A) \frac{\sigma^2}{N}.$$

It is instructive to consider the consequences of taking the observations from an underlying model given by $\mu(x) = f(x)$ for a wide choice of $f(x)$. Thus suppose that $f(x)$ is expressible in a standard Fourier representation

$$f(x) = \sum_{h \in \mathbb{Z}^d} \alpha(h) e^{2\pi i h^t x} \quad (7.3)$$

where $\alpha(h) = \int_{[0,1]^d} f(x) e^{-2\pi i h^t x} dx$. Sufficient conditions for uniform convergence are well known and omitted.

Under suitable conditions the set $\{e^{2\pi i h^t x} : h \in \mathbb{Z}^d\}$ forms an orthogonal basis of $L^2(\mathbb{R}^d)$ and through the Fourier transform there is a one-to-one mapping from $l^2(\mathbb{Z}^d)$ to $L^2(\mathbb{R}^d)$. We may thus fix an order on \mathbb{Z}^d and write the Fourier decomposition of $f(x)$ as the scalar product of the infinite complex vectors

$$\begin{aligned} Z_\infty(x) &= (1, \dots, e^{2\pi i h^t x}, \dots, e^{-2\pi i h^t x}, \dots)^t \\ \alpha_\infty &= (\alpha(0), \dots, \alpha(h), \dots, \alpha(-h), \dots)^t \end{aligned}$$

so that

$$f(x) = Z_\infty(x)^t \alpha_\infty.$$

Suppose we have a Fourier model A and a one-generator lattice design $D \equiv L$ with N points is chosen such that (D, A) is completely orthogonal. If we observe without error, then the observation vector is

$$Y = (f(x_1), \dots, f(x_N))^t = Z_\infty \alpha_\infty$$

where the k th row of Z_∞ is $Z_\infty(x_k)^t$. Then, using the orthogonality, the least squared estimator is

$$\hat{\alpha} = (Z^* Z)^{-1} Z^* Y = \frac{1}{N} Z^* Y = \frac{1}{N} Z^* Z_\infty \alpha_\infty.$$

Then

$$\begin{aligned} \frac{1}{N} Z^* Z_\infty &= \frac{1}{N} \left(\sum_{x \in L} e^{2\pi i(-h+k)^t x} \right)_{h \in A, k \in \mathbf{Z}^d} \\ &= (\delta_{h,k})_{h \in A, k \in \mathbf{Z}^d} \end{aligned}$$

where

$$\delta_{h,k} = \begin{cases} 1 & \text{if } -h + k \in L^\perp \\ 0 & \text{otherwise} \end{cases}$$

or equivalently

$$\delta_{h,k} = \begin{cases} 1 & \text{if } k \in L_h^\perp \\ 0 & \text{otherwise.} \end{cases}$$

This analysis generalises the Nyquist folding to lattices. The fitted model, when there is no error, is

$$\hat{\mu}(x) = \sum_{h \in A} \left(\sum_{k \in L_h^\perp} \alpha(k) \right) e^{2\pi i x^t h}.$$

Employing the L^2 orthogonality of the Fourier terms over $[0, 1]^d$ we have the integrated square error

$$I_2 = \int_{[0,1]^d} (\hat{Y}(x) - f(x))^2 dx = \sum_{h \in A} \left(\sum_{k \in L_h^\perp; k \neq h} \alpha(k) \right)^2 + \sum_{k \in \mathbf{Z}^d - A} \alpha(k)^2. \quad (7.4)$$

If there is observation error then I_2 represents the bias term and the full integrated mean square error is

$$IMSE = I_1 + I_2.$$

It is clear from (7.4) that I_2 is unbounded unless further conditions are added to the Fourier coefficients $\alpha(k)$ over and above the L^2 -condition: $\sum_{k \in \mathbf{Z}^d} \alpha(k)^2 < \infty$.

A natural condition is

$$\sum_{k \in \mathbf{Z}^d} |\alpha(k)| < \infty$$

which is equivalent to absolute convergence of $f(x)$. Stronger conditions still are the $E_\alpha(c)$ conditions used in the integration theory of lattices (see Niederreiter, 1992, Definition 5.1). Further research is needed to find designs which guard against growth of the bias term I_2 . In such work the relationship between the design $D \equiv L$ and the source of biases as given by (7.4) should play a major part and the trade off between I_1 and I_2 , will be relevant.

Summary

Lattice designs for screening experiments are introduced in this chapter. A multi-dimensional model can be embedded into one dimension using the one-dimensional structure of one-generator lattices over the unitary hypercube. Thus the allowed

analysis with the fast Fourier transform, in the specific case a power spectrum calculation, can be carried out in one dimension and the result can be translated back to the multidimensional space exploiting the inverse of the one-generator lattice rule. Inspection of the peaks in the spectrum is used to detect significant effects.

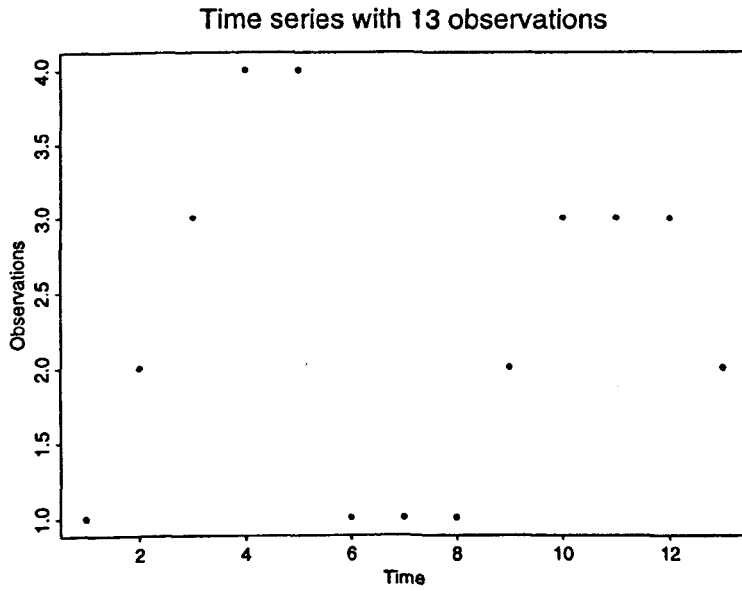


Figure 7.1: Observed values at the $L_{(1,5),13}$ design points.

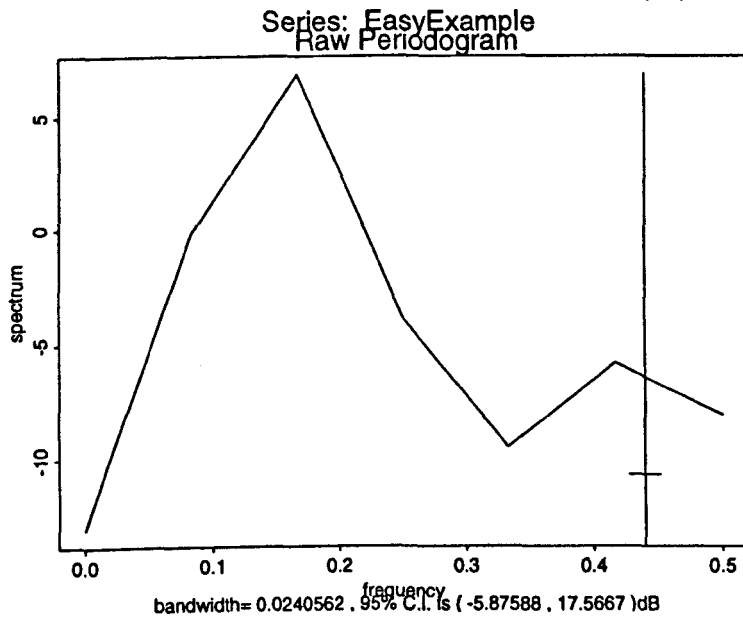


Figure 7.2: Power spectrum augmented by the mean.

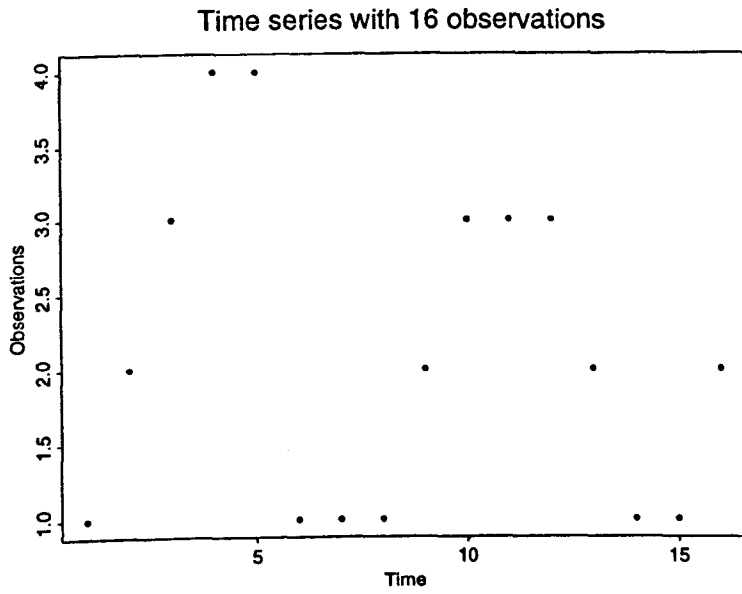


Figure 7.3: Observed values at the $L_{(1,5),16}$ design points.

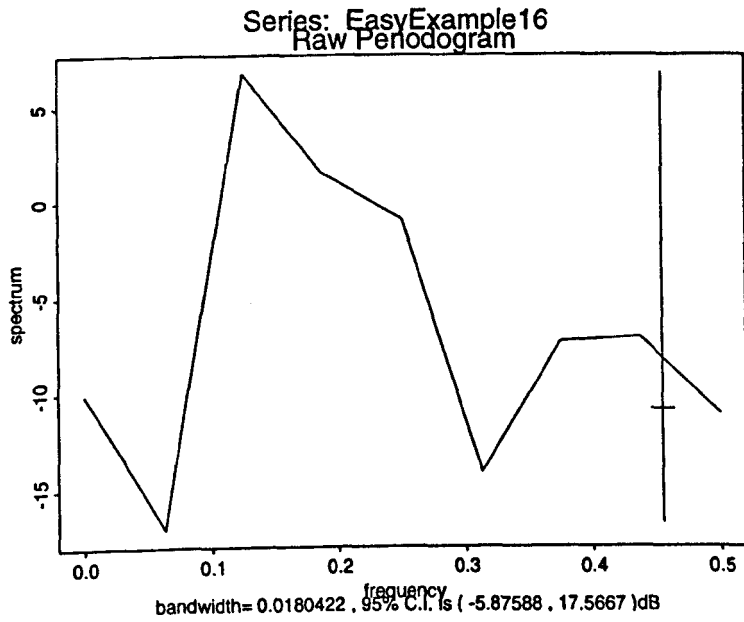


Figure 7.4: Power spectrum augmented by the mean.

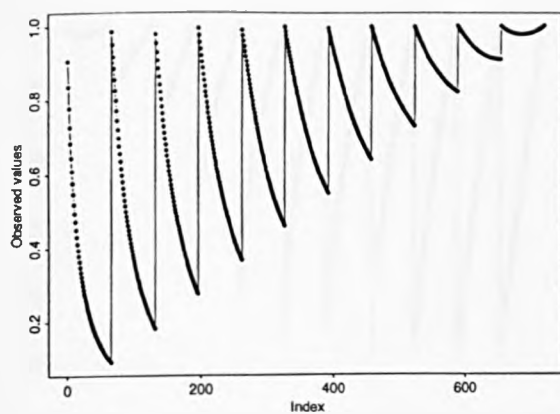


Figure 7.5: Observed values at $L_{(1,61,11),721}$ from $x_1^{x_3}$.

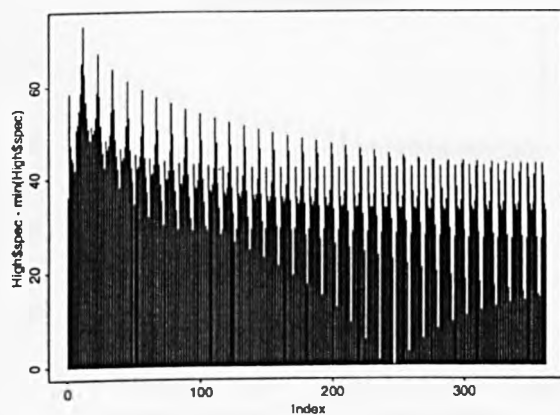


Figure 7.6: Power spectrum for data from $x_1^{x_3}$.

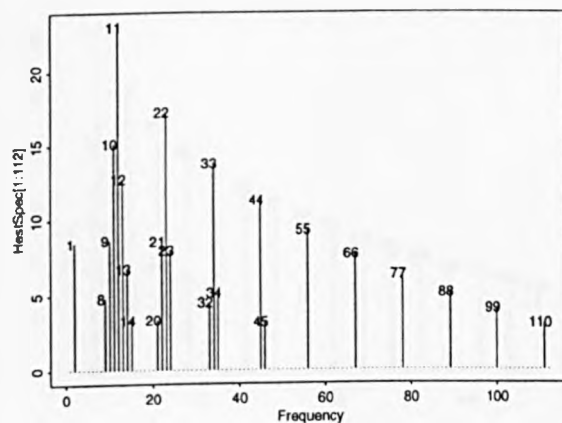


Figure 7.7: Frequencies with highest spectrum for data from $x_1^{x_3}$.

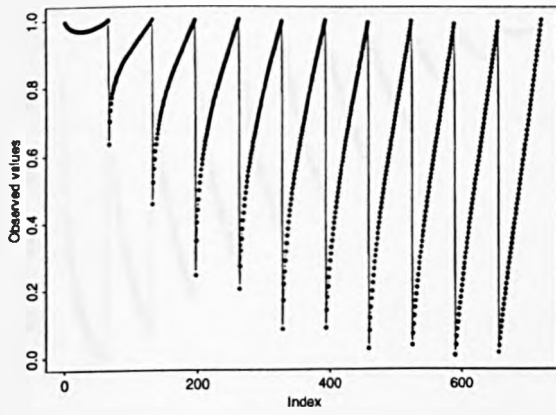


Figure 7.8: Observed values at $L_{(11,61,1),721}$ from x_1^{23} and power spectrum.

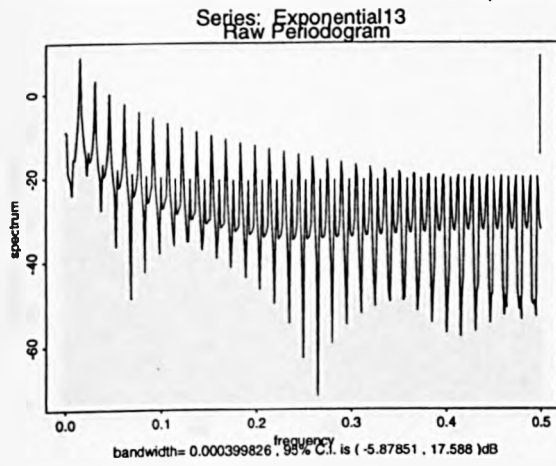


Figure 7.9: Power spectrum for data from x_1^{23} at $L_{(11,61,1),721}$.

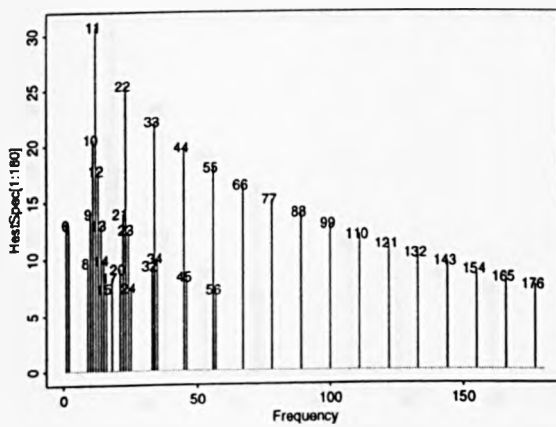


Figure 7.10: Frequencies with highest spectrum for data from x_1^{23} .

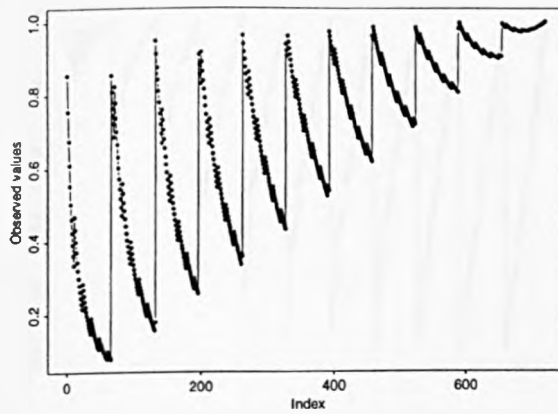


Figure 7.11: Observed values at $L_{(1,61,11),721}$ from $x_1^{x_3+1x_2}$.

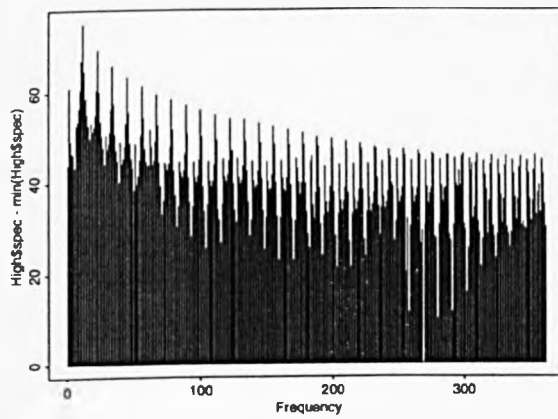


Figure 7.12: Power spectrum for values at $L_{(1,61,11),721}$ from $x_1^{x_3+1x_2}$.

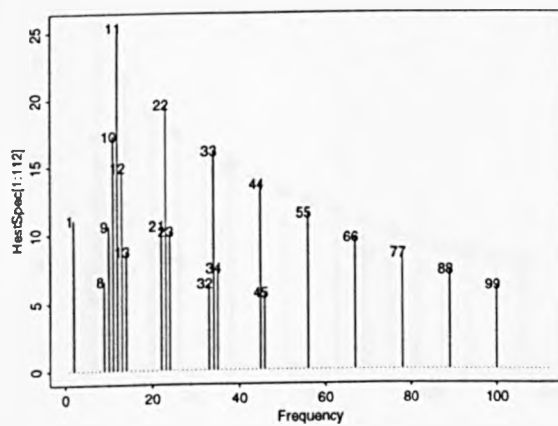


Figure 7.13: Frequencies with highest spectrum for data from $x_1^{x_3}$ at $L_{(1,61,11),721}$.

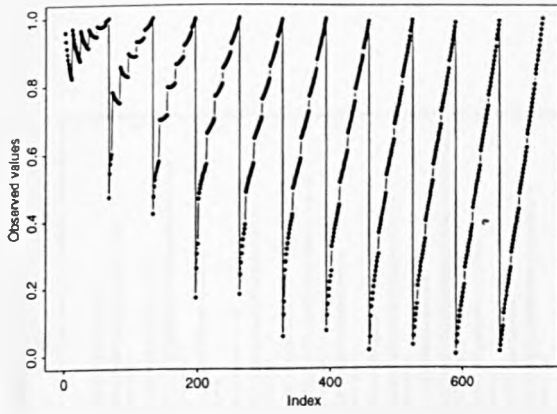


Figure 7.14: Observed values at $L_{(11,61,1),721}$ from $x_1^{x_3+.1x_2}$.

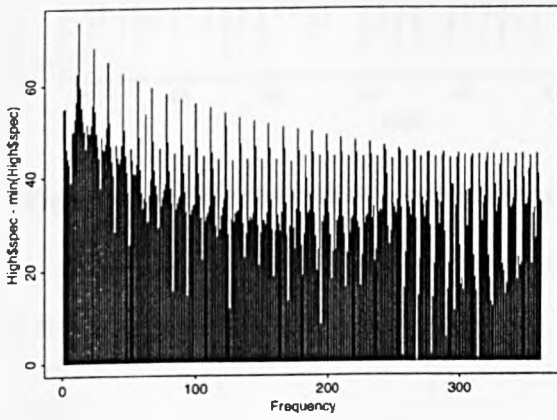


Figure 7.15: Power spectrum for values at $L_{(11,61,1),721}$ from $x_1^{x_3+.1x_2}$.

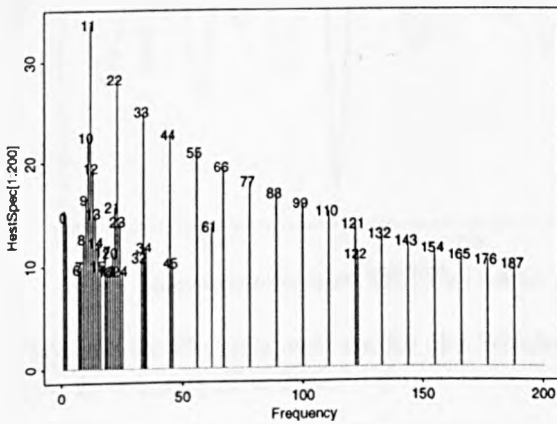


Figure 7.16: Frequencies with highest spectrum for data from $x_1^{x_3}$.

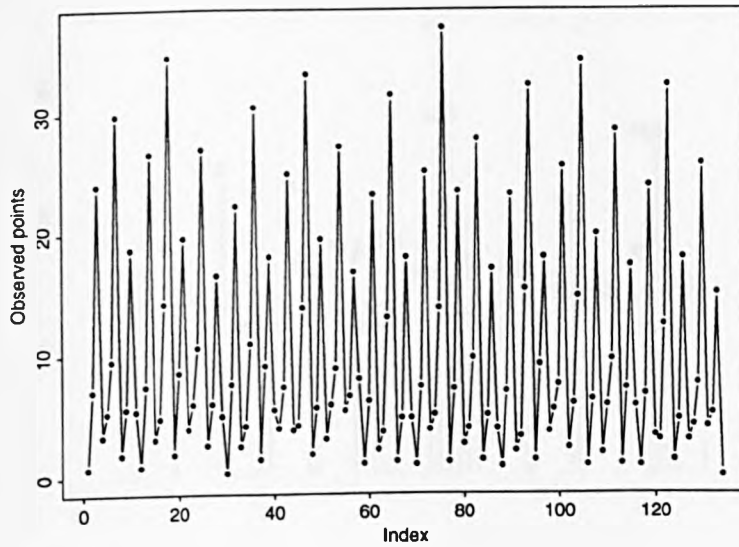


Figure 7.17: Observed values and power spectrum for the Welch et al. function.

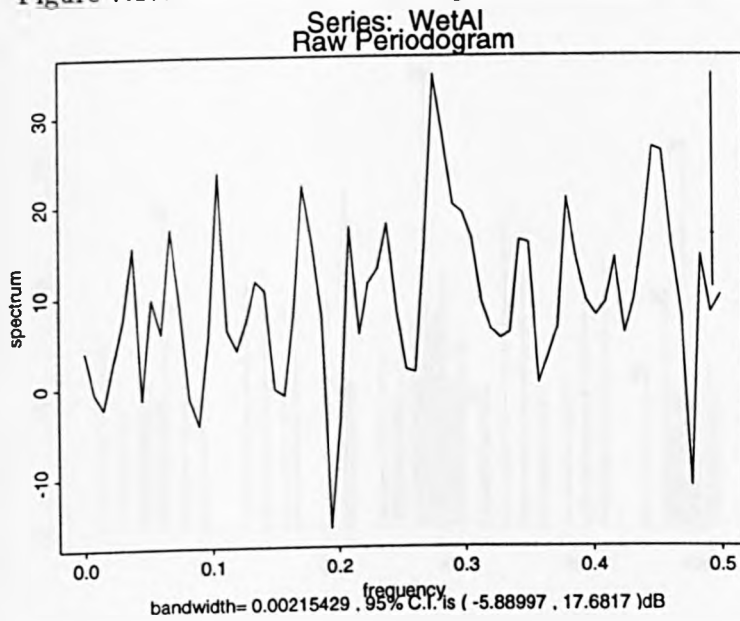


Figure 7.18: Power spectrum for the Welch et al. function for the lattice design with $g_i = 2i - 1$ and $N = 134$.

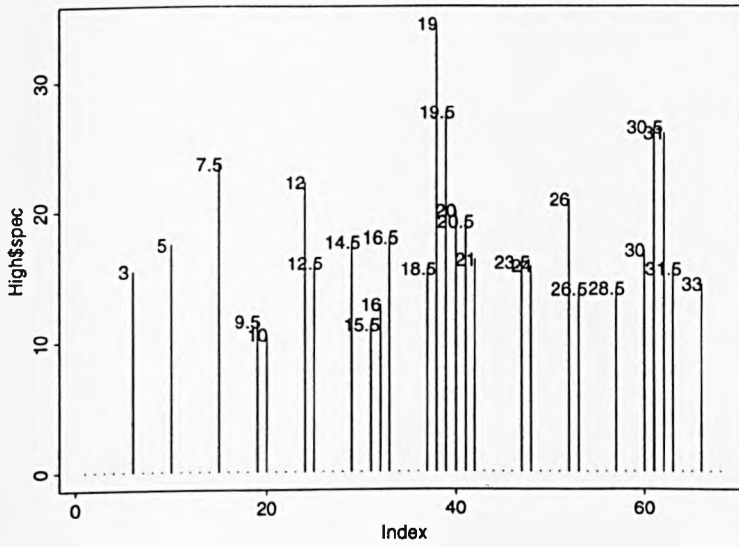


Figure 7.19: Frequencies with highest spectrum for the Welch et al. function.

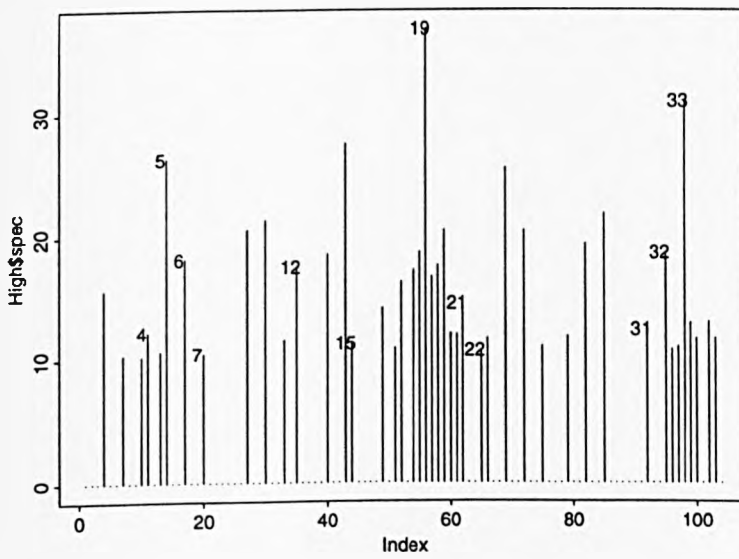


Figure 7.20: Frequencies with highest spectrum for the Welch et al. function for the lattice design with $g_i = 3i - 2$ and $N = 207$.

Part III

Algebraic Identifiability for Fourier Models

Chapter 8

Applications of Gröbner bases to Fourier models

In the present chapter we show how the algebraic techniques for identifiability apply to Fourier models. To do that we implement a version of the Buchberger algorithm that works over simple algebraic extensions of the rational numbers. We verify the compatibility of the two theories: the orthogonality of lattice designs for Fourier models and the algebraic computational approach to identifiability and then we consider less structured designs. The chapter is organised as follows. In Sections 8.1 and 8.2 Fourier models and lattice designs respectively are rewritten as polynomials. In Section 8.3 we describe the modifications to the Buchberger algorithm needed to work with complex numbers. Our code is to be made available via anonymous ftp at `lancelot.dima.unige.it` and can be found in Appendix .2. In Section 8.4 we present some examples.

8.1 Fourier models as polynomials

Let A be a subset of integer vectors as from Definition 21 of Chapter 4 and let $E(Y)$ be the corresponding model

$$\begin{aligned} E(Y(x)) &= \theta_0 + \sqrt{2} \sum_{h \in A^+} [\theta_h \sin(2\pi h^t x) + \phi_h \cos(2\pi h^t x)] \\ &= \alpha_0 + \sum_{h \in A^+} [\beta_h e^{2\pi i h^t x} + \delta_h e^{-2\pi i h^t x}], \end{aligned} \quad (8.1)$$

where as usual $x \in [0, 1]^d$, $\theta_0, \theta_h, \phi_h \in \mathbb{R}$ and $\alpha_0, \beta_h, \delta_h \in \mathbb{C}$ where \mathbb{R} and \mathbb{C} are the real numbers and the complex numbers respectively.

Using standard formulae one can rewrite Fourier models as polynomials. This is made clear by an example. Let us consider the following two-dimensional Fourier model:

$$\begin{aligned} E(Y(x_1, x_2)) &= \theta_0 + \sqrt{2}(\theta_1 \sin(2\pi x_1) + \phi_1 \cos(2\pi x_1)) \\ &+ \sqrt{2}(\theta_2 \sin(4\pi x_2) + \phi_2 \cos(4\pi x_2)) \\ &+ \sqrt{2}(\theta_3 \sin(2\pi(x_1 + x_2)) + \phi_3 \cos(2\pi(x_1 + x_2))). \end{aligned} \quad (8.2)$$

A frequency set A^+ is $\{(1, 0), (0, 2), (1, 1)\}$. Using the addition and subtraction formulae for sine and cosine it can be rewritten as

$$\begin{aligned} E(Y(x_1, x_2)) &= \theta_0 + \sqrt{2}(\theta_1 \sin(2\pi x_1) + \phi_1 \cos(2\pi x_1)) \\ &+ \sqrt{2}(\theta_2 \sin(2\pi x_2) \cos(2\pi x_2) + \phi_2(2 \cos(2\pi x_2)^2 - 1)) \\ &+ \sqrt{2}(\theta_3(\sin(2\pi x_1) \cos(2\pi x_2) + \cos(2\pi x_1) \sin(2\pi x_2)) \\ &\quad + \phi_3(\cos(2\pi x_1) \cos(2\pi x_2) - \sin(2\pi x_1) \sin(2\pi x_2))). \end{aligned} \quad (8.3)$$

Substituting the following identities in (8.3)

$$\begin{aligned} s_1 &:= \sin(2\pi x_1), \\ c_1 &:= \cos(2\pi x_1), \\ s_2 &:= \sin(2\pi x_2), \text{ and} \\ c_2 &:= \cos(2\pi x_2), \end{aligned}$$

the Fourier model (8.2) can be written as the following set of polynomial equations:

$$\begin{cases} E(Y(c_1, c_2, s_1, s_2)) = \theta_0 + \sqrt{2}(\theta_1 s_1 + \phi_1 c_1) + \sqrt{2}(2\theta_2 s_2 c_2 + \phi_2(2c_2^2 - 1)) \\ \quad + \sqrt{2}(\theta_3(s_1 c_2 + c_1 s_2) + \phi_3(c_1 c_2 - s_1 s_2)) \\ c_1^2 + s_1^2 = 1 \\ c_2^2 + s_2^2 = 1 \end{cases}$$

where the equations $c_1^2 + s_1^2 = 1$ and $c_2^2 + s_2^2 = 1$ give the sin/cos relations.

The conversion from the Fourier form to the polynomial form and vice-versa can be performed in several symbolic calculus packages. For example in Maple it is obtained by the commands `expand`, `combine` and `subs` as we show next with reference to the above example:

```
> # X=2*Pi*x;
> # From Fourier form to polynomial form
> Example:=subs(cos(X[1])=c[1], sin(X[1])=s[1], cos(X[2])=c[2], sin(X[2])=s[2],
> expand(theta[0] + sqrt(2)*(theta[1]*sin(X[1]) + phi[1]*cos(X[1]))
> + sqrt(2)*(theta[2]*sin(2*X[2])+phi[2]*cos(2*X[2]))
> + sqrt(2)*(theta[3]*sin(X[1]+X[2])+phi[3]*cos(X[1]+X[2])));
```

$$\begin{aligned} \text{Example} &:= \theta_0 + \sqrt{2}\theta_1 s_1 + \sqrt{2}\phi_1 c_1 + 2\sqrt{2}\theta_2 s_2 c_2 + 2\sqrt{2}\phi_2 c_2^2 \\ &\quad - \sqrt{2}\phi_2 + \sqrt{2}\theta_3 s_1 c_2 + \sqrt{2}\theta_3 c_1 s_2 + \sqrt{2}\phi_3 c_1 c_2 - \sqrt{2}\phi_3 s_1 s_2 \end{aligned}$$

```
> # From polynomial form to Fourier form
> combine(subs(c[1]=cos(X[1]), s[1]=sin(X[1]), c[2]=cos(X[2]), s[2]=sin(X[2]),
> Example), trig);
```

$$\begin{aligned} &\theta_0 + \sqrt{2}\theta_1 \sin(X_1) + \sqrt{2}\phi_1 \cos(X_1) + \sqrt{2}\theta_2 \sin(2X_2) \\ &\quad + \sqrt{2}\phi_2 \cos(2X_2) + \sqrt{2}\theta_3 \sin(X_1 + X_2) + \sqrt{2}\phi_3 \cos(X_1 + X_2) \end{aligned}$$

Note that these commands transform exponents of polynomials into frequencies of Fourier models (see also Example 8.2 and Section 6). To fully benefit from this correspondence we have to interpret algebraically the trigonometric condition $\sin(x)^2 + \cos(x)^2 = 1$. We do this by considering the polynomial ring modulo the ideal generated by the following polynomials:

$$c_j^2 + s_j^2 - 1 : j = 1, \dots, d.$$

Theorem 58 *There is a one-to-one correspondence between the following two sets:*

$$\mathcal{M} := \left\{ \sum_{h \in A} \alpha_h e^{2\pi i h^t x} : A \subset \mathbb{Z}^d, A \text{ finite}, x = (x_1, \dots, x_d) \text{ and } \alpha_h \in k(i) \right\}, \text{ and}$$

$$\mathcal{P} := k(i)[c_1, \dots, c_d, s_1, \dots, s_d] / (c_1^2 + s_1^2 - 1, \dots, c_d^2 + s_d^2 - 1)$$

where $k(i)$ is the simple algebraic extension of the coefficients field k with the imaginary unit i .

Proof. First we observe that \mathcal{M} and \mathcal{P} are rings with the usual operations of addition and multiplication. Then we exhibit two ring morphisms

$$\phi : \mathcal{M} \longrightarrow \mathcal{P} \quad \text{and} \quad \psi : \mathcal{P} \longrightarrow \mathcal{M}$$

such that $\psi \circ \phi = id_{\mathcal{P}}$ and $\phi \circ \psi = id_{\mathcal{M}}$. Let $1 \leq j, k \leq d$; the function ϕ is defined over the elementary forms through the De Moivre's identity as follows and then extended by linearity to the whole ring

$$e^{2in\pi x_j} = \cos(2n\pi x_j) + i \sin(2n\pi x_j) = (\cos(2\pi x_j) + i \sin(2\pi x_j))^n$$

and thus

$$\phi(e^{2in\pi x_j}) = (c_j + is_j)^n$$

where $c_j = \phi(\cos(2\pi x_j))$ and $s_j = \phi(\sin(2\pi x_j))$. Moreover this gives

$$\begin{aligned} \cos(2n\pi x_j) &= \frac{1}{2} ((\cos(2\pi x_j) + i \sin(2\pi x_j))^n + (\cos(2\pi x_j) - i \sin(2\pi x_j))^n) \\ &= \frac{1}{2} ((c_j + is_j)^n + (c_j - is_j)^n), \text{ and} \\ \sin(2n\pi x_j) &= \frac{1}{2i} ((\cos(2\pi x_j) + i \sin(2\pi x_j))^n - (\cos(2\pi x_j) - i \sin(2\pi x_j))^n) \\ &= \frac{-i}{2} ((c_j + is_j)^n - (c_j - is_j)^n) \end{aligned}$$

and thus

$$\begin{aligned} \phi(\cos(2n\pi x_j)) &= \frac{1}{2} ((c_j + is_j)^n + (c_j - is_j)^n) \\ \phi(\sin(2n\pi x_j)) &= \frac{-i}{2} ((c_j + is_j)^n - (c_j - is_j)^n). \end{aligned}$$

Conversely ψ follows from the following identities:

$$\begin{aligned} \psi(s_j^n) = \sin^n(2\pi x_j) &= \left(\frac{e^{i2\pi x_j} - e^{-i2\pi x_j}}{2i} \right)^n = \frac{-i^n}{2^n} \sum_{l=0}^n \binom{n}{l} (-1)^l e^{2i\pi x_j(2l-n)}, \text{ and} \\ \psi(c_j^n) = \cos^n(2\pi x_j) &= \left(\frac{e^{i2\pi x_j} + e^{-i2\pi x_j}}{2} \right)^n = \frac{1}{2^n} \sum_{l=0}^n \binom{n}{l} e^{2i\pi x_j(2l-n)}. \end{aligned}$$

Observe that $c_j + is_j$ is invertible in \mathcal{P} . Simple but tedious computations prove $\psi \circ \phi = id_{\mathcal{P}}$ and $\phi \circ \psi = id_{\mathcal{M}}$. We note that sum of Fourier models corresponds to sum of polynomials: for $\phi(e^{2i\pi x_j}) = c_j + is_j$ and $\phi(e^{2i\pi x_k}) = c_k + is_k$ we have that

$$\phi(e^{2i\pi x_j} + e^{2i\pi x_k}) = c_j + c_k + i(s_j + s_k),$$

and for the product we have the following identities:

$$\begin{aligned}\phi(e^{i(2\pi x_j + 2\pi x_k)}) &= (c_j + is_j)(c_k + is_k) = (c_j c_k - s_j s_k) + i(c_j s_k + s_j c_k), \text{ and} \\ \phi(e^{i(2\pi x_j - 2\pi x_k)}) &= (c_j + is_j)(c_k - is_k) = (c_j c_k + s_j s_k) + i(c_j s_k - s_j c_k).\end{aligned}$$

□

The set of complete Fourier models as defined in Bates *et al.* (1995) [4] is a subset of \mathcal{M} , for example $e^{+2\pi h^t x} \in \mathcal{M}$ is not a complete Fourier model.

8.2 Polynomial representation of lattice designs

Recall Theorem 35 from Chapter 5 and consider the two-dimensional lattice $L_{(1,5),13}$. It is orthogonal for the Fourier model with frequencies

$$A^+ = \{(1, 0), (0, 1), (1, 1), (1, -1), (2, 0), (0, 2)\}$$

since the following numbers are distinct (mod 13) from each other and from their additive inverse (mod 13)

$$\begin{aligned}(1, 0)(1, 5)^t &\equiv 1 \pmod{13}, \\ (0, 1)(1, 5)^t &\equiv 5 \pmod{13}, \\ (1, 1)(1, 5)^t &\equiv 6 \pmod{13}, \\ (1, -1)(1, 5)^t &\equiv -4 \pmod{13}, \\ (2, 0)(1, 5)^t &\equiv 2 \pmod{13}, \text{ and} \\ (0, 2)(1, 5)^t &\equiv -3 \pmod{13}.\end{aligned}$$

According to the transformations in the proof of Theorem 58 the set of frequencies A^+ corresponds to the following set of polynomials:

$$\{ c_1 + is_1, c_2 + is_2, (c_1 + is_1)(c_2 + is_2), \\ (c_1 + is_1)(c_2 - is_2), (c_1 + is_1)^2, (c_2 + is_2)^2 \}.$$

Next we write the lattice design $L_{(1,5),13}$ as a system of polynomial equations. Consider the first coordinate of L , $x_1 \in [0, 1[$. It is in one-to-one correspondence with the set of points

$$\left\{ \frac{2\pi j}{13} : j = 0, \dots, 12 \right\}$$

and it can be interpreted as a set of equidistant angles in a Gaussian plane. Thus the set of the first coordinates of L is in one-to-one correspondence with the 13 complex roots of the unit. In particular it is in one-to-one correspondence with the solutions of the following system of complex equations:

$$\begin{cases} (c_1 + is_1)^{13} = 1 \\ c_1^2 + s_1^2 = 1, \end{cases}$$

where $c_1 = \cos(2\pi x_1)$, $s_1 = \sin(2\pi x_1)$ for $x_1 \in [0, 1)$. Similarly for the second coordinate we have

$$\begin{cases} (c_2 + is_2)^{13} = 1 \\ c_2^2 + s_2^2 = 1. \end{cases}$$

Finally the equation

$$c_2 + is_2 = (c_1 + is_1)^5$$

links the two sets of coordinates according to the lattice rule.

In general the d -dimensional lattice generated by (g_1, \dots, g_d) and with N points, where the g_j 's and N are mutually prime, corresponds to the following system of complex polynomials with $3d - 1$ equations and $2d + 1$ variables:

$$\begin{cases} (c_1 + is_1)^N = 1, & \dots, & (c_d + is_d)^N = 1 \\ (c_2 + is_2)^{g_1} = (c_1 + is_1)^{g_2} \\ \vdots \\ (c_d + is_d)^{g_1} = (c_1 + is_1)^{g_d} \\ c_1^2 + s_1^2 = 1, & \dots, & c_d^2 + s_d^2 = 1. \end{cases}$$

8.3 Gröbner basis technology

Theoretically speaking the algebraic theory as exposed in Chapter 3 works for any design providing we can determine the design ideal. This is always possible if we work over a field that includes all the values assumed by the design points. Most Gröbner bases packages (for example CoCoA and Maple) are built to work with rational numbers. As already noticed this does not prove restrictive for the application of the algebraic theory to classical polynomial regression models. That is the use of design points with rational coordinates is not a restriction since in real experiments rational numbers are good approximations of irrational ones.

In the trigonometric case a complication arises from the fact that most of the time sine and cosine of rational numbers are irrational numbers. Let us consider one such number, say α . The standard algebraic solution is to work not in $\mathbb{Q}(\alpha)[x]$ but in its isomorphic image $\mathbb{Q}[x, \alpha]/f(\alpha)$, where $f(\alpha)$ is the minimal polynomial of α . For example $\mathbb{Q}(i)[x] \simeq \mathbb{Q}[x, t]/(t^2 + 1)$ and $\mathbb{Q}(\sqrt{2})[x] \simeq \mathbb{Q}[x, t]/(t^2 - 2)$.

We describe here a variant of the Buchberger algorithm that works on $\mathbb{Q}[x, t]$ and, given an ideal $I(D) \subset \mathbb{Q}[x, t]$ computes its Gröbner basis on $\mathbb{Q}[x, t]/(t^2 + 1) \simeq \mathbb{Q}(i)[x]$. This version, based on special treatment of some indeterminates, requires adaptations of standard methods which are not explicitly found in the literature. The two key points are as follows:

- 1) the elements of $\mathbb{Q}[x, t]$ are interpreted as elements of $\mathbb{Q}[x, t]/(t^2 + 1)$, and hence the relation $t^2 = -1$ can be exploited. In particular any polynomial we are dealing with is normalised in such a way the degree of the variable t is at most 1.
- 2) The indeterminate t has to behave as a coefficient.

Adjustments to the treatment of the ring $\mathbb{Q}[x, t]$:

- a) the term-ordering τ on $\mathbb{Q}[x]$ is extended to a term-ordering on $\mathbb{Q}[x, t]$ and thus to $\mathbb{Q}(i)[x]$ in such a way that $x_1^{\alpha_1} \dots x_d^{\alpha_d} t^\alpha >_\tau t^\beta$ for all $\alpha_1, \dots, \alpha_d, \alpha, \beta$ non-negative integers.
- b) A term $x_1^{\alpha_1} \dots x_d^{\alpha_d} t^\alpha$ divides a term $x_1^{\beta_1} \dots x_d^{\beta_d} t^\beta$ if and only if $x_1^{\alpha_1} \dots x_d^{\alpha_d}$ divides $x_1^{\beta_1} \dots x_d^{\beta_d}$. Note that in this case $x_1^{\alpha_1} \dots x_d^{\alpha_d} t^\alpha$ divides $x_1^{\beta_1} \dots x_d^{\beta_d} t^\beta$ for all α, β non negative integers. That is t behaves like a coefficient.

c) The leading coefficient of a polynomial of the form

$$ax_1^{\alpha_1} \cdots x_d^{\alpha_d} t + bx_1^{\alpha_1} \cdots x_d^{\alpha_d} + \text{terms smaller (w.r.t. } \tau) \text{ than } x_1^{\alpha_1} \cdots x_d^{\alpha_d},$$

is $at + b$ and its leading term is $x_1^{\alpha_1} \cdots x_d^{\alpha_d}$.

d) When it is necessary to invert a polynomial $at + b$ (for example in the S-polynomial and remainder procedures), the inverse is computed as $\frac{b-ta}{a^2+b^2}$ (the usual complex inverse).

Then, we perform the Buchberger algorithm on the ring $\mathbb{Q}[x, t]$ with respect to the ordering defined in a) with the following modifications :

- 1) throughout the Buchberger algorithm, the divisibility tests are performed in accordance with b) and the leading coefficients are computed as defined in c).
- 2) The generators of $I(D)$ are divided by $t^2 + 1$.
- 3) Throughout the remainder procedure, if we multiply some polynomial by t , then we divide the result by $t^2 + 1$.

It is easy to see that the set of polynomials computed by this version of the Buchberger algorithm is a Gröbner basis for $I(D)$ over $\mathbb{Q}[x, t]/(t^2 + 1)$. Note that any simple algebraic extension of the rational numbers may be dealt with using the above technique. Another method of computing Gröbner bases over an algebraic extension of the rationals is to add the minimal polynomial to the generators and run on them the Buchberger algorithm with some specialized strategy. For details, see Mora and Traverso, 1992, Preprint).

Let $I \subset \mathbb{Q}(i)[x_1, x_2, x_3]$ be the ideal generated by $((i^3 + 2)x_1^2x_2 - x_3^3, ix_2^3 - x_3^3)$ and let us consider $\text{tdeg}(x_1 > x_2 > x_3)$. Then we compute the Gröbner basis of the ideal

$$J := (x_1^2x_2t^3 + 2x_1^2x_2 - x_3^3, x_2^3t - x_3^3) \subset \mathbb{Q}[x_1, x_2, x_3, t]$$

with respect to the term-ordering

$$x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3} t^\alpha > x_1^{\beta_1} x_2^{\beta_2} x_3^{\beta_3} t^\beta \Leftrightarrow \begin{cases} x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3} >_{\text{tdeg}} x_1^{\beta_1} x_2^{\beta_2} x_3^{\beta_3} \\ \text{or} \\ x_1^{\alpha_1} x_2^{\alpha_2} x_3^{\alpha_3} = x_1^{\beta_1} x_2^{\beta_2} x_3^{\beta_3} \text{ and } \alpha > \beta. \end{cases}$$

The generators of J are divided by $t^2 + 1$, giving

$$\{f_1, f_2\} := \{-x_1^2x_2t + 2x_1^2x_2 - x_3^3, x_2^3t - x_3^3\}.$$

The leading coefficients of f_1 and f_2 are $2 - t$ and t respectively. Their leading terms are $x_1^2x_2$ and x_2^3 respectively. Their S-polynomial is

$$\begin{aligned} \text{SPoly}(f_1, f_2) &= x_2^2(2-t)^{-1}(-x_1^2x_2t + 2x_1^2x_2 - x_3^3) - x_1^2t^{-1}(x_2^3t - x_3^3) \\ &= t^{-1}x_1^2x_3^3 - (2-t)^{-1}x_3^3x_2^2 \\ &= -x_1^2x_3^3t - \frac{(t+2)}{5}x_3^3x_2^2. \end{aligned}$$

Completing the Gröbner basis gives

$$G := \{x_1^2x_2 - 1/5x_3^3t - 2/5x_3^3, x_2^3 + x_3^3t, x_1^2x_3^3 - 2/5x_2^2x_3^3t + 1/5x_2^2x_3^3\} \subset \mathbb{Q}[x_1, x_2, x_3, t],$$

as to say

$$G := \{x_1^2x_2 - \frac{i+2}{5}x_3^3, x_2^3 + x_3^3i, x_1^2x_3^3 + \frac{-2i+1}{5}x_2^2x_3^3\} \subset \mathbb{Q}(i)[x_1, x_2, x_3].$$

8.4 Examples

In this section we present three examples: the $L_{(1,5),13}$ design, the design obtained by the union of the $L_{(1,5),13}$ and the design D in Table 8.1 that does not have a group structure and finally the design described in Subsection 8.4.3. In this section the coefficient field is a suitable simple algebraic extension of the rational numbers.

8.4.1 Example: $L_{(1,5),13}$

With this example we test how the algebraic procedure recaptures the aliasing structure arising from the group nature of lattice design. As we have seen in Section 8.2 the ideal corresponding to $L_{(1,5),13}$ is generated by the following polynomials:

$$\left\{ \begin{array}{l} (c_1 + is_1)^{13} - 1 \\ c_1^2 + s_1^2 - 1 \\ (c_2 + is_2)^{13} - 1 \\ c_2^2 + s_2^2 - 1 \\ c_2 + is_2 - (c_1 + is_1)^5. \end{array} \right.$$

Thus we work with polynomials with rational coefficients in the 5 ($= 4 + 1$) indeterminates s_1, c_1, s_2, c_2, i . With $\text{tdeg}(c_1 > c_2 > s_1 > s_2 > i)$ the Gröbner basis of the design ideal is :

$$\left\{ \begin{array}{l} c_1^2 + s_1^2 - 1, \quad c_2^2 + s_2^2 - 1, \\ c_1 c_2 s_1 + 1/4 c_2 s_1 + 1/4 c_1 s_2 - 1/2 c_2 s_2, \\ c_1 s_1^2 - 1/2 s_2^2 - 1/4 c_1 + 1/4, \\ c_1 c_2 s_2 + 1/2 c_1 s_1 - 1/4 c_2 s_1 + 1/4 c_1 s_2, \\ c_2 s_1 s_2 - 1/4 c_1 c_2 - 1/2 s_1^2 - 1/4 s_1 s_2 + 1/4, \\ c_2 s_2^2 - 1/2 s_1^2 - 1/4 c_2 + 1/4, \\ c_2 s_1^2 + 1/4 c_1 c_2 - 1/4 s_1 s_2 - 1/2 s_2^2 - 1/2 c_2 + 1/4, \\ s_1^3 - 1/2 c_2 s_2 - 3/4 s_1, \\ c_1 s_2^2 + 1/4 c_1 c_2 - 1/2 s_1^2 + 1/4 s_1 s_2 - 1/2 c_1 + 1/4, \\ c_1 s_1 s_2 + 1/4 c_1 c_2 - 1/4 s_1 s_2 + 1/2 s_2^2 - 1/4, \\ s_1^2 s_2 - 1/4 c_2 s_1 - 1/4 c_1 s_2 - 1/2 c_2 s_2 - 1/2 s_2, \\ s_1 s_2^2 - 1/2 c_1 s_1 - 1/4 c_2 s_1 + 1/4 c_1 s_2 - 1/2 s_1, \\ s_2^3 + 1/2 c_1 s_1 - 3/4 s_2 \quad \}. \end{array} \right.$$

Let L_t be the set of (tdeg)-leading terms of the ideal $I(D)$ so-obtained

$$c_1^2, c_2^2, c_1 c_2 s_1, c_1 s_1^2, c_1 c_2 s_2, c_2 s_1 s_2, c_2 s_2^2, c_2 s_1^2, s_1^3, c_1 s_2^2, c_1 s_1 s_2, s_1^2 s_2, s_1 s_2^2, s_2^3.$$

Finally the estimable terms are represented by those terms not divisible by any element in L_t (see Part I) and thus we have

$$1, c_1, c_2, s_1, s_2, c_1 c_2, c_1 s_1, c_2 s_1, s_1^2, c_1 s_2, c_2 s_2, s_1 s_2, s_2^2.$$

Following Theorem 58 from the set of estimable terms we recapture the trigonometric terms

$$1, e^{2\pi i x_1}, e^{2\pi i x_2}$$

given by $1, c_1, s_1, c_2, s_2$, and

$$e^{2\pi i(x_1+x_2)}, e^{2\pi i(x_1-x_2)}$$

given by $c_1c_2, c_1s_2, c_2s_1, s_1s_2$. They correspond to the first order terms that is the frequency set

$$A^+ = \{(1, 0), (0, 1), (1, 1), (1, -1)\}.$$

The monomials c_2s_2 and c_1s_1 give

$$\frac{1}{2} (e^{-2\pi ix_1} + e^{2\pi ix_1}) = \frac{1}{2} \sin(2\pi 2x_1), \quad \frac{1}{2} (e^{-2\pi ix_2} + e^{2\pi ix_2}) = \frac{1}{2} \sin(2\pi 2x_2)$$

and from s_1^2 and s_2^2 we get

$$\frac{1}{2} (e^{-2\pi i2x_1} + e^{2\pi i2x_1}) = \frac{1}{2} \cos(2\pi 2x_1), \quad \frac{1}{2} (e^{-2\pi i2x_2} + e^{2\pi i2x_2}) = \frac{1}{2} \cos(2\pi 2x_2)$$

that together give the second order frequencies $(2, 0)$ and $(0, 2)$. Thus we have found the model in Equation 8.3.

Using the `lex` term-ordering we obtain the following set of estimable terms:

$$1, s_2, s_2^2, s_2^3, s_2^4, s_2^5, s_2^6, s_2^7, s_2^8, s_2^9, s_2^{10}, s_2^{11}, s_2^{12}$$

from the following Gröbner basis:

$$GB = \left\{ \begin{array}{l} c_1 - 128s_2^8 + 256s_2^6 - 160s_2^4 + 32s_2^2 - 1, \\ s_1 - 16s_2^5 + 20s_2^3 - 5s_2, \\ c_2 - 2048s_2^{12} + 6144s_2^{10} - 6912s_2^8 + 3584s_2^6 - 840s_2^4 + 72s_2^2 - 1, \\ s_2^{13} - 13/4s_2^{11} + 65/16s_2^9 - 39/16s_2^7 + 91/128s_2^5 - 91/1024s_2^3 + 13/4096s_2 \end{array} \right\}.$$

Next we show how with `lex` we can estimate the model A^+ of Equation 8.2. In Maple the model is written as follows:

```
> Mod:=theta[0]+theta[1]*cos(X)+theta[2]*sin(X)+theta[3]*cos(Y)+theta[4]*sin(Y)
> +theta[5]*cos(X+Y)+theta[6]*sin(X+Y)+theta[7]*cos(X-Y)+theta[8]*sin(X-Y)
> +theta[9]*cos(2*X)+theta[10]*sin(2*X)+theta[11]*cos(2*Y)+theta[12]*sin(2*Y):
```

where θ_j ($j = 0, \dots, 12$) is the parameter vector to be estimated. We write it in polynomial form with the following command:

```
> PolMod:=subs(cos(X)=c1,sin(X)=s1,cos(Y)=c2,sin(Y)=s2,expand(Mod)).
```

Then we divide it out by GB and find the estimable polynomial aliased with $PolMod$ and of minimum degree with respect to the `lex` term-ordering using the Maple command `normalf`:

```
> Ali :=normalf( PolMod,GB,[c1,c2,s1,s2,i],plex);
Ali := (-256 theta_8 - 2816 theta_12) s2^9 + (64 theta_6 + 576 theta_8 + 2816 theta_12) s2^7
+ (theta_4 - 7 theta_6 - 9 theta_8 - 3 theta_10 - 11 theta_12 + 5 theta_2) s2^5
+ (1280 theta_9 + 128 theta_1 + 6912 theta_3) s2^3
+ (-1120 theta_9 - 256 theta_1 - 32 theta_5 - 3584 theta_3) s2 + 2048 theta_3 s2^12
```

$$\begin{aligned}
& + (-512\theta_9 - 6144\theta_3) s^2^{10} + \theta_0 + \theta_9 + \theta_{11} + \theta_1 + \theta_3 + \theta_5 + \theta_7 \\
& + 1024\theta_{12} s^2^{11} + (400\theta_9 + 160\theta_1 + 48\theta_5 + 8\theta_7 + 840\theta_3) s^2^4 \\
& + (-50\theta_9 - 32\theta_1 - 18\theta_5 - 8\theta_7 - 2\theta_{11} - 72\theta_3) s^2^2 \\
& + (-112\theta_6 - 432\theta_8 - 1232\theta_{12} + 16\theta_2) s^2^5 \\
& + (4\theta_{10} + 56\theta_6 + 120\theta_8 + 220\theta_{12} - 20\theta_2) s^2^3.
\end{aligned}$$

A linear system links the 13 coefficients of the polynomial so obtained (let us call them ϕ_j , $j = 0, \dots, 12$) to the 13 coefficients to be estimated. This is usually the case since normalf operates linearly on the coefficients. As usual we estimate the ϕ_j 's ($j = 0, \dots, 12$) and solve the linear system to get an estimate of the θ_j 's ($j = 0, \dots, 12$).

8.4.2 Example: the union of $L_{(1,5),13}$ and D

We can compute the Gröbner basis for the ideal corresponding to the design D in Table 8.1 over $\mathbb{Q}(c_1, c_2, s_1, s_2)$. With the tdeg term-ordering we obtain the following Gröbner basis:

$$\left\{ \begin{array}{l} c_2 s_2, c_2 s_1 + s_1 s_2 - s_1, \\ c_1 s_1, c_2^2 + s_2^2 - 1, \\ c_1 c_2 + c_1 s_2 - c_1 - c_2 - s_2 + 1, \\ c_1^2 + s_1^2 - 1, \\ c_1 s_2^2 - c_1 s_2 - s_2^2 + s_2, \\ s_2^3 - s_2, s_1 s_2^2 - s_1 s_2, \\ s_1^2 s_2 - s_1 s_2, s_1^3 - s_1 \end{array} \right\}.$$

None of the polynomials in the design ideals for $L_{(1,5),13}$ and D involves the imaginary unit. Thus we use the standard Buchberger algorithm to calculate the reduced Gröbner basis of the union of D and $L_{(1,5),13}$, which corresponds to the intersection of the two design ideals. We have the following set of 21 ($= 13 + 9 - 1$) estimable terms:

$$1, c_1, c_2, s_1, s_2, c_1 s_2, s_1^2, s_1 s_2, s_2^2, s_1^3, s_1^2 s_2, s_1 s_2^2, s_2^3, s_1^4, s_1^3 s_2, s_1^2 s_2^2, s_1 s_2^3, s_2^4, s_1 s_2^4, s_2^5, s_2^6.$$

Table 8.3 shows to which trigonometric terms the estimable set corresponds. As expected there is the frequency set A estimable with the $L_{(1,5),13}$ alone. No other frequency is fully estimable by the bigger design but effects of other frequencies are recaptured: for example $\sin(2\pi 3x)$ is estimable but not $\cos(2\pi 3x)$. In the interpretation of Table 8.3 one needs to bear in mind that linear non-singular transformations of estimable parameters are estimable. As a consequence constants (even those involving the imaginary unit) are not reported and neither are terms that already appear in Table 8.3 read from top to bottom.

One can test whether a frequency of interest that is a sin/cos pair can be added to the set of fully estimable frequencies without losing the identifiability by exploiting the aliasing/confounding relation mentioned in Section 8.1. For example $\cos(2\pi 3x)$ cannot be added to the set A since the terms of the remainder $Rem(\phi(\cos(2\pi 3x)), G)$,

where G is the Gröbner basis for the 21-point design, are already involved in the definition of A .

8.4.3 Example: the design F

Let F be the 3-dimensional design in Table 8.2. Because of the point F_8 we work over $\mathbb{Q}(\frac{\sqrt{2}}{2})$ and thus we consider $\mathbb{Q}[c_1, c_2, c_3, s_1, s_2, s_3, a]/(a^2 - 1/2)$, where a plays the role of $\frac{\sqrt{2}}{2}$ (see Section 8.3). With $\text{tdeg}(c_1 > c_2 > c_3 > s_1 > s_2 > s_3 > a)$ the set of estimable terms is

$$1, c_1, c_2, c_3, s_3, c_1 c_2, c_1 c_3, c_2 c_3,$$

which gives only the intercept and the frequency $(0, 0, 1)$ as fully estimable. Using Maple we find that the polynomial in $\mathbb{Q}(\frac{\sqrt{2}}{2})[c_1, c_2, c_3, s_1, s_2, s_3]/I(F)$ aliased with the following model:

$$\begin{aligned} &\theta_0 + \theta_1 \sin(X_2 + X_3) + \psi_1 \cos(X_2 + X_3) + \theta_2 \sin(X_1 + X_3) \\ &\quad + \psi_2 \cos(X_1 + X_3) + \theta_3 \sin(X_1 + X_2) + \psi_3 \cos(X_1 + X_2) \\ &\quad + \theta_4 \sin(X_1 + X_2 + X_3) + \psi_4 \cos(X_1 + X_2 + X_3) \end{aligned}$$

is

$$\begin{aligned} &(\psi_2 + \psi_4) c_1 c_3 + (\psi_1 + \psi_4) c_2 c_3 - \psi_4 c_1 - \psi_4 c_2 + (\theta_2 + \theta_3) c_1 s_3 + \theta_0 \\ &\quad + \psi_4 + \frac{1}{2} (-5\psi_4 - 2\theta_1 - \theta_3 - \theta_2 - \psi_2 - \psi_3 - \psi_1) s_3 \sqrt{2} \\ &\quad + (-3\psi_4 + \theta_4) s_3 - \psi_4 c_3 + (\psi_3 + \psi_4) c_1 c_2 + \psi_4 s_3. \end{aligned}$$

From the last equation we have that the parameters $\theta_0, \psi_1, \theta_1, \psi_2, \psi_3, \psi_4, \theta_4$ are estimable together with the linear combination $\theta_2 + \theta_3$. This gives the intercept and the frequencies $(0, 1, 1)$ and $(1, 1, 1)$ as fully estimable.

The examples of Subsections 8.4.2 and 8.4.3 show that, from a statistical point of view, a limitation of the application of the algebraic identifiability procedure to Fourier models is that the saturated model returned does not always make sense because it may include for example a sine term for a certain frequency but not the cosine term. Nevertheless the models we can identify can be considered as belonging to a more general class of Fourier regression models than those defined in Bates *et al.* (1995) [4]: specifically that defined in Theorem 58. This limitation cannot be overcome since it is intrinsic in the nature of Fourier models.

To conclude we note that with ad hoc modifications the technique described in this paper can be applied to any class of statistical models that forms a ring and for which a theorem analogous to Theorem 58 holds. An example is the set of exponential models of the form

$$\left\{ \sum_{h \in A} \beta e^{h^t x} : A \subset \mathbb{Z}_+^d, A \text{ finite and } \beta \in \mathbb{Q} \right\}$$

that is in one-to-one correspondence with $\mathbb{Q}[x]$. Also Haar functions are subject of further research.

Summary

In this chapter we apply the algebraic technique in the first part of the thesis to the Fourier models of the Part II. The following change of variables $s = \sin(2\pi x)$, $c = \cos(2\pi x)$ together with the equation representing the fundamental trigonometric identity $c^2 + s^2 = 1$ allows us to map over to the polynomial case. In particular we give a new complex version of the Buchberger algorithm for computation of Gröbner bases. The theory of orthogonality of lattice designs for Fourier models is tested on some examples and shows some correspondence between the results obtained by the lattice methods and the Gröbner basis method, but also some differences. The possibility to extend the application to other ring of function models such as Haar functions, splines, wavelets, ... is mentioned.

	x_1	x_2
D_1	0	0
D_2	1/4	0
D_3	2/4	0
D_4	3/4	0
D_5	0	1/4
D_6	0	2/4
D_7	0	3/4
D_8	1/4	1/4
D_9	2/4	1/4

Table 8.1: The design D

	x_1	x_2	x_3
F_1	0	0	0
F_2	1/2	0	0
F_3	0	1/2	0
F_4	0	0	1/2
F_5	1/2	1/2	0
F_6	1/2	0	1/2
F_7	0	1/2	1/2
F_8	1/8	1/8	1/8

Table 8.2: The design F

1	1
c_1	$e^{2\pi i x} + e^{-2\pi i x}$
s_1	$e^{2\pi i x} - e^{-2\pi i x}$
c_2	$e^{2\pi i y} + e^{-2\pi i y}$
s_2	$e^{2\pi i y} - e^{-2\pi i y}$
$c_1 s_2$	$e^{2\pi i(x+y)} - e^{-2\pi i(x+y)} - (e^{2\pi i(x-y)} - e^{-2\pi i(x-y)})$
s_1^2	$e^{2\pi i 2x} + e^{-2\pi i 2x}$
$s_1 s_2$	$e^{2\pi i(x+y)} + e^{-2\pi i(x+y)} - (e^{2\pi i(x-y)} + e^{-2\pi i(x-y)})$
s_2^2	$e^{2\pi i 2y} + e^{-2\pi i 2y}$
s_1^3	$e^{2\pi i 3x} - e^{-2\pi i 3x}$
$s_1^2 s_2$	$e^{2\pi i(2x+y)} - e^{-2\pi i(2x+y)} + (e^{2\pi i(2x-y)} + e^{-2\pi i(2x-y)})$
$s_1 s_2^2$	$e^{2\pi i(x+2y)} - e^{-2\pi i(x+2y)} + (e^{2\pi i(x-2y)} + e^{-2\pi i(x-2y)})$
s_2^3	$e^{2\pi i 3y} - e^{-2\pi i 3y}$
s_1^4	$e^{2\pi i 4x} + e^{-2\pi i 4x}$
$s_1^3 s_2$	$e^{2\pi i(3x+y)} + e^{-2\pi i(3x+y)} - (e^{2\pi i(3x-y)} + e^{-2\pi i(3x-y)})$
$s_1^2 s_2^2$	$e^{2\pi i(2x+2y)} + e^{-2\pi i(2x+2y)} + (e^{2\pi i(2x-2y)} + e^{-2\pi i(2x+2y)})$
$s_1 s_2^3$	$e^{2\pi i(x+3y)} + e^{-2\pi i(x+3y)} - (e^{2\pi i(x-3y)} + e^{-2\pi i(x-3y)})$
s_2^4	$e^{2\pi i 4y} + e^{-2\pi i 4y}$
$s_1 s_2^4$	$e^{2\pi i(x+4y)} - e^{-2\pi i(x+4y)} + (e^{2\pi i(x-4y)} - e^{-2\pi i(x-4y)})$
s_2^5	$e^{2\pi i 5y} - e^{-2\pi i 5y}$
s_2^6	$e^{2\pi i 6y} + e^{-2\pi i 6y}$

Table 8.3: Estimable terms by $L_{(1,5),13} \cup D$

Part IV

**Conclusions and Further
Research**

The thesis represents part of a continuing active and fast developing research programme and brings together a volume of research conducted both by the author alone and as part of a research team. This means that throughout the thesis there are lines of research development which point to current and planned research and areas which are only, as yet, in the nature of speculation. We summarise these in note form below.

1. Fan theory. The theory of fan is currently under investigation. Beyond this there is the problem of classifying the fans in terms of the basic geometric structure of the designs themselves. This amounts to a total classification of all experimental designs by the estimability of polynomial models, and would imply a complete solution to the confounding/aliasing of factorial models.

2. Fourier and other rings. All results for polynomials including the classification in 1 above should be extended to other rings of functions. For Fourier this means a large outgrowth from Chapter 8. Haar functions, wavelettes, Gaussian and exponential kernels are all examples of particularly useful model classes.

3. Complexity. The material on generator construction in Chapter 6 can be considered as a kind of complexity theory as model dimension tends to infinity with a class of models. Linking this to identifiability more closely (also for polynomial and other rings) may lead to a new complexity theory within algebraic geometry itself. The link with fractal dimension may be woven into such a theory.

4. Non-linear models. Section 3.4 is a truncated version of current research. All of the above theory ought to be extendible to differential rings by adjoining differential operators both ordinary and partial. These methods are the subject of intensive research within the control theory and related areas of system theory, particularly the so-called compartmental models. When such models are linear (as differential equations) Laplace transforms can turn them into models as in Section 3.4. The non-linear theory still awaits serious development. In particular extensions to models which are rational in the parameters should be possible and by approximation extension to non-polynomial model should be feasible as well.

5. Stochastic models and statistical theory. The models in this thesis can be considered as models for the mean of a statistical model. It is a major challenge to lift the theory to a full probabilistic model while retaining the algebraic theory in a common operational environment. A start has been made by the author, coauthors and colleagues in two works in progress. The connection to Bayesian analysis and influence diagrams and to the algebraic theory of the exponential family are promising and it is being studied in collaboration with R. Settini and J.Q. Smith. See also Riccomagno and Wynn (1997) [59].

A nice aspect of the algebraic theory to identifiability is its applicability to real case studies. See for example the paper by Holliday, Pistone, Riccomagno and Wynn (1996) [37] where data describing a part of a motor engine are considered. In that paper the idea of a fan is used first. The paper titled "Multi-strain species modelling via differential algebra reduction" in collaboration with L. White is a second step in this direction. A multi-strain species model can be described by a system of ordinary polynomial differential equations with respect to time combined with some linear algebraic equations which we refer to as conservative laws. Iterative suitable differentiations with respect to time allow us to construct a system of polynomial equations where the differentials are considered indeterminates. For example

consider the system

$$\begin{aligned} A: \quad \dot{x}_1 &= \alpha_1 x_2 + \beta_1 x_1 \\ B: \quad \dot{x}_2 &= \alpha_2 x_2 + \beta_2 x_1 \\ C: \quad y &= x_1 + x_2 \end{aligned}$$

where the x_i 's, $i = 1, 2$, and their derivatives are assumed difficult to know and y and its derivatives are easy to measure. The aim is to give some estimates of the parameters α_i and β_i ($i = 1, 2$). Consider the polynomial system of equations $A, B, C, \dot{A}, \dot{B}, \dot{C}$ in the indeterminates $\dot{x}_1, \ddot{x}_2, \dot{x}_1, \dot{x}_2, x_1, x_2, \ddot{y}, \dot{y}, y$ by eliminating the x_i variables and their derivatives by the system, for example computing the Gröbner basis of the system with respect to the plex ordering we get the following equations involving only y and its derivatives and the parameters

$$\ddot{y} + (\alpha_1 \beta_2 - \beta_1 \alpha_2) y - (\alpha_1 + \beta_2) \dot{y}.$$

Bibliography

- [1] W. W. Adams and P. Lounstaunau. *An Introduction to Gröbner Bases*. Graduate Studies in Mathematics. AMS, 1994.
- [2] J. P. Barbot and N. Pantalos. Using symbolic-calculus for singularly perturbed nonlinear-systems. *Lecture notes in Control and Information Sciences*, 165:40–49, 1991.
- [3] R. Bates, R. Buck, E. Riccomagno, and H. Wynn. Experimental design and observation for large systems (with discussion). *J. Royal Stats. Soc. B*, 58(1):77–94, 1995.
- [4] R. Bates, E. Riccomagno, R. Schwabe, and H. Wynn. Lattices and dual lattices in optimal experimental design for Fourier models. In K.-T. Fang and F. J. Hickernell, editors, *Proceedings of workshop on Quasi-Monte Carlo Methods and Their Applications (preliminary results)*, pages 1–16, Honk-Kong, 1995. Submitted CSDA.
- [5] R. A. Bates, E. Riccomagno, R. Schwabe, and H. Wynn. Fast Fourier emulators based on space-filling lattices. Freie Universität Berlin, Fachbereich Mathematik und Informatik, Serie A · Mathematik, Preprint Nr. A/23/95, 1995.
- [6] M. Bayram, J. P. Bennet, and M. C. Dewar. Using computer algebra to determine rate constants in biochemistry. *Acta biotheoretica*, 41(1-2):53–62, 1993.
- [7] E. Becker, M. Marinari, T. Mora, and C. Traverso. Shape lemma. In *Proc. ISSAC'94*, pages 131–140. ACM, 1994.
- [8] T. Becker and H. Weispfenning, Volker (in cooperation with Kredel. *Gröber Bases. A Computational Approach to Commutative Algebra*. Springer -Verlag, New-York, 1991.
- [9] N. L. Biggs. *Discrete Mathematics*. Claredon Press, Oxford, 1989. rev. ed.
- [10] P. Bloomfield. *Fourier Analysis of Time Series: An Introduction*. Wiley, New-York, 1976.
- [11] D. Brillinger. *Time Series, Data Analysis and Theory*. Holden-Day, Inc., San Francisco, 1981. Expanded Edition.
- [12] M. Caboara, G. de Dominicis, and L. Robbiano. Multigraded Hilbert function and Buchberger algorithm. In Y. Lakshman, editor, *Proc. ISSAC'96*, pages 72–78. ACM, 1996.

- [13] M. Caboara, G. Pistone, E. Riccomagno, and H. Wynn. The fan of an experimental design. Submitted, May 1997.
- [14] M. Caboara and E. Riccomagno. An algebraic computational approach to the identifiability of Fourier models. *JSC*, In press.
- [15] M. Caboara and L. Robbiano. Families of ideals in statistics. In *Proc. ISSAC'97*, page in press. ACM, 1997.
- [16] M. Caboara and C. Traverso. The powerful Buchberger algorithm for modules. Preprint, 1996.
- [17] A. Capani and G. Niesi. *CoCoA User's Manual*. Department of Mathematics, University of Genova., 1995. Available via anonymous ftp from `lancelot.dima.unige.it`.
- [18] G. Casella and R. L. Berger. *Statistical Inference*. Wadsworth & Brooks/Cole, California, 1992.
- [19] M. Chappell and K. Godfrey. Structural identifiability of the parameters of a nonlinear batch reactor model. *Mathematical Biosciences*, 108:241–251, 1992.
- [20] B. Char, K. Geddes, G. Gonnet, B. Leong, and M. Monogan. *MAPLE V Library Reference Manual*. Springer-Verlag, New York, 1991.
- [21] S. Collart and D. Kalkbrener, M. amd Mall. Converting bases with the gröbner walk. *J. Symb. Comput.*, 24(3/4):465–469, 1997.
- [22] J. H. Conway and N. J. A. Sloane. *Sphere Packings, Lattices and Groups*. Springer-Verlag, New York, 1992.
- [23] D. R. Cook and L. A. Thibodeau. Marginally restricted d -optimal designs. *J. Amer. Statist. Assoc.*, 75:366–371, 1980.
- [24] D. Cox, J. Little, and D. O'Shea. *Ideal, Varieties, and Algorithms*. Springer-Verlag, New York, 1992.
- [25] H. Dette and G. Haller. Optimal discriminating. In *New Developments and Applications in Experimental Design*, IMS Lecture Notes-Monograph Series. AMS/SIAM/IMS Joint Summer Research Conference in the Mthematical, 1997.
- [26] P. Diaconis, R. L. Graham, and B. Sturmfels. Primitive partition identities. *Combinatorics*, 2:173–192, 1996.
- [27] P. Diaconis and B. Sturmfels. Algebraic algorithms for sampling from conditional distributions. *Preprint SC 93-17, 1993, ZIB Berlin*, 1993.
- [28] D. Eisenbud. *Commutative Algebra with a View Toward Algebraic Geometry*, volume 150 of *Springer Graduate Texts in Mathematics*. Springer-Verlag, New-York, 1995.
- [29] K. Fang and Y. Wang. *Number-theoretic Methods in Statistics*. Chapman & Hall, London, 1994.

- [30] P. Fitzpatrick. On the key equation. *IEEE Transactions on Information Theory*, 41(5):1290–1302, 1995.
- [31] R. Fontana, G. Pistone, and M.-P. Rogantin. Algebraic analysis and generation of two-level designs. *Stats. Appl.*, 9, 1:0–0 (In press), 1997.
- [32] A. Giovagnoli, F. Pukelsheim, and H. P. Wynn. Group invariant orderings and experimental design. *Journal of Statistical Planning and Inference*, 17:159–171, 1987.
- [33] A. Giovagnoli and H. P. Wynn. G -majorization with applications to matrix orderings. *Linear algebra and its applications*, 67:111–135, 1985.
- [34] A. Giovagnoli and H. P. Wynn. *Optimal design*, 1988. 3rd E.C.A.S. course, Design of Experiment.
- [35] K. Hagglof, P. O. Lindberg, and L. Svensson. Computing global minima to polynomial optimization problems using Groebner bases. *Journal of Global Optimization*, 7(2):115–125, 1995.
- [36] P. Hoel. Minimax distance designs in two dimensional regression. *Ann. Math. Statist.*, 36:1097–1106, 1965.
- [37] T. Holliday, G. Pistone, E. Riccomagno, and H. Wynn. The application of algebraic geometry to the design and analysis of experiments: A case study. in press, 1997.
- [38] N. I. Ioakimidis and E. G. Anastasselou. Computer-based manipulation of systems of equations in elasticity problems with Groebner bases. *Computer Methods In Applied Mechanics an Engineering*, 110(1-2):103–111, 1993.
- [39] J. Kiefer. Optimum experimental designs. *J. Royal Statistical Society, Series B.*, 21:272–304, 1959.
- [40] J. Kiefer and J. Wolfowitz. Optimum design in regression problem. *Ann. Math. Statist.*, 30:271–294, 1959.
- [41] A. Kobilinsky. Complex linear models and cyclic designs. *Linear Algebra and Its Applications*, 127:227–282, 1990.
- [42] V. Koval and R. Schwabe. Uniformly distributed sequences as experimental designs innonparametric regression estimation by orthogonal series. Technical Report 1924, Technische Hochschule Darmstadt, Fachbereich Mathematik, 1997.
- [43] V. Kurotschka. A general approach to optimum design of experiments with qualitative and quantitative factors. In J. Ghosh and J. Roy, editors, *Statistics: Applications and New Directions: Proceedings of the Indian Statistical Institute Golden Jubilee International Conference, 1981*, volume 3, pages 353–368, 1984.
- [44] L. Ljung and T. Glad. On global identifiability by arbitrary model parametrizations. *Automatica*, 30(2):265–276, 1994.

- [45] M. Marinari, H. Möller, and T. Mora. Gröbner bases of ideals defined by functionals with an application to ideals of projective points. *Applicable Algebra in Engineering, Communication and Computing*, 4(2):103–145, 1993.
- [46] M. Marinari, H. Möller, and T. Mora. Gröbner duality. Technical Report 312, Università di Genova, Dipartimento di Matematica, 1996. Preprint.
- [47] T. Mora. An introduction to commutative and non-commutative Gröbner bases. *Theoretical Computer Science*, 134(1):131–173, 1994.
- [48] T. Mora. Notes on polynomial system solving, 1996. Lecture, ISSAC'96 Conference, Zurich.
- [49] T. Mora and L. Robbiano. The Gröbner fan of an ideal. *JSC*, 6:183–208, 1988.
- [50] H. Niederreiter. *Random Number Generation and Quasi-Monte Carlo Methods*. CBMS-NFS, SIAM, Philadelphia, 1992.
- [51] A. B. Owen. Lattice sampling revisited: Monte Carlo variance of means over randomized orthogonal arrays. *Ann. Statist.*, 22, 1994.
- [52] G. Pistone, E. Riccomagno, and H. Wynn. Applications of Gröbner bases in statistics, 1996. A course of four informal lectures hold at the Department of Statistics, University of Warwick, April-May 1996.
- [53] G. Pistone and H. P. Wynn. Generalised confounding with Gröbner bases. *Biometrika*, 83(3):653–666, 1996.
- [54] F. Pukelsheim. *Optimal Design of Experiments*. Wiley, New York, 1993.
- [55] E. Rafajłowicz and W. Myszka. When product type experimental design is optimal? brief survey and new results. *Metrika*, 39:321–333, 1992.
- [56] M. Reid. *Undergraduate Algebraic Geometry*, volume 12 of *London Mathematical Society Student Texts*. Cambridge University Press, Cambridge, 1994.
- [57] E. Riccomagno. Rational noncommutative formal power series and iterated integral representation of a class of Ito processes. *Bollettino UMI, VII. Ser. B*, 10(1):25–50, 1996.
- [58] E. Riccomagno, R. Schwabe, and H. Wynn. Lattice-based optimum design for Fourier regression. *Annals of Statistics*, 1997. In press.
- [59] E. Riccomagno and H. Wynn. Computational algebraic geometry in industrial experimental design. In C. P. Kitsos and L. Edler, editors, *Proceedings of the International Conference on Industrial Statistics: Aims and Computational Aspects*, pages 193–197, Athens, August 1997. Physica-Verlag.
- [60] L. Robbiano. Term orderings on the polynomial rings. In *EUROCAL'85*, number 204 in LNCS, pages 513–517, 1985.
- [61] L. Robbiano and M. Rogantin. Factorial designs and distracted fractions. Technical Report 344, Dipartimento di Matematica, U. Genova, 1997. Submitted to Proceedings of the International Conference “33 years of Gröbner basis”.

- [62] J. Sacks, W. J. Welch, T. J. Mitchell, and H. P. Wynn. Design and analysis of computer experiments (with discussion). *Statist. Sci.*, 4:409–435, 1989.
- [63] R. Schwabe. Model robust experimental design in the presence of interactions: The orthogonal case. In T. M. M. Publ., editor, *PROBASTAT'94. Proc. Int. Conf. Math. Statist., Smolenice 1994*, volume 7, 1994.
- [64] R. Schwabe. Experimental designs for linear models with higher order interaction terms. In V. Mammitzsch and H. Schneeweibb, editors, *Proc. 2nd Gauss Symp., Conf B: Statist. Sci., München, 1993*, pages 281–288, Berlin, 1995. De-Gruyter.
- [65] R. Schwabe. Optimal designs for additive linear models. *Statistics*, 27:267–278, 1996.
- [66] R. Schwabe. *Optimum Design for Multi-Factor Models*, volume 113 of *Lectures Notes in Statistics*. Springer, New York, 1996.
- [67] P. Shi and K. Fang. Optimal U-design under multi-criteria for Fourier regression models. In F. J. H. Kai-Tai Fang, editor, *Proceeding's Workshop on Quasi-Monte Carlo Methods and Their Applications*, 1995.
- [68] S. Silvey. *Optimal Design*. Chapman & Hall, London, 1980.
- [69] I. Sloan and S. Joe. *Lattice Methods for Multiple Integration*. Oxford Science Publications, Oxford, 1994.
- [70] B. Sturmfels. *Gröbner Bases and Convex polytopes*, volume Volume 8. Ed. AMS, Providence R I, 1995. University Lecture Series.
- [71] C. Traverso. Hilbert functions and the Buchberger algorithm. *Journal of Symbolic Computations*, 22(4):355–376, 1996.
- [72] T. Vafiadis and N. Karcanias. The solution of the cover problems using Groebner basis techniques. In *2nd IEEE Mediterranean Symposium in New Direction on Control and Automation, 1994 Crete*, June 1994.
- [73] W. W. S. Wei. *Time series Analysis. Univariate and Multivariate Methods*. Addison-Wesley, California, 1990.
- [74] W. J. Welch, R. J. Buck, J. Sacks, H. P. Wynn, T. J. Mitchell, and M. D. Morris. Screening, predicting, and computer experiment. *Technometrics*, 34(1):15–25, 1992.
- [75] H. S. Wilf. *Generatingfunctionology*. Academic Press, Inc., Boston, 1990.
- [76] S. Yeşilyurt and A. Patera. Surrogates for numerical simulations; optimization of eddy-promoter heat exchangers. *Comp. Meth. in Appl. Mech. and Eng.*, (in press).

Part V
Appendices

.1 Computer algebra packages

There are many computer algebra systems which have implemented a package to work with Gröbner bases. We use two of them in the thesis: Maple and CoCoA. Maple, by the University of Waterloo, Canada, is a general purpose package quite fast, simple to use and with an helpful online help. The Gröbner package of Maple is called by the command

```
> with(grobner);
    [finduni, finite, gbasis, gsolve, leadmon, normalf, solvable, spoly]
```

The above are the eight functions available in the Gröbner package. Next we describe the ones we mostly use. The function *gbasis*($F, X, termorder$) computes the reduced Gröbner basis of the ideal F introduced as a list of polynomials in the indeterminates specified in the list X and with respect to the term-ordering *termorder*. There are two possible term-orderings in Maple: *tdeg*, that is the total degree reverse lexicographic ordering and *plex*, the lexicographic ordering. The initial ordering is the one in which the indeterminates are given in the list of indeterminates. All the “letters” in the input basis and not in the list of variables are treated as constant. This implies that computation with free parameters is possible in Maple. This is a general feature of the Gröbner package in Maple that is not available for example in CoCoA.

The function *normalf*(*poly*, F, X) computes the remainder of the polynomial *poly* with respect to the ideal basis F which has to be a Gröbner basis with respect to the indeterminates X . A term-ordering either *plex* or *tdeg* can be specified.

The function *gsolve*(F, X) return the list of solutions of the system F with respect to the variables X . The computation is done via elimination theory.

Examples of the use of those functions can be found throughout the thesis.

CoCoA (COmputations in COmmutative Algebra) is a special purpose package for Gröbner basis computation developed at the University of Genova, Italy. It is obtainable for free via anonymous ftp at lancelot.dima.unige.it. The drawback of CoCoA is that, since it is designed primarily for researchers in algebraic geometry and commutative algebra, it is at times not as intuitive to use as Maple. But it allows more refined computations such as Gröbner bases for modules and Hilbert function computations. We used none of them in the thesis. CoCoA has three main advantages with respect to Maple. First, it is faster and it computes Gröbner bases of ideals that Maple cannot handle. Second, it allows custom defined term-orderings via the specification of a suitable $d \times d$ integer matrix where d is the number of indeterminates. Third, it allows easier manipulation of some algebraic structures such as ideals.

The working field has to be specified in advance. The coefficient field could be the set of rational numbers or a finite field. For example in a session starting with the line

```
Use T:=Q[xyz], DegRevLex;
```

we are considering polynomials in the three indeterminates x, y, z with rational coefficients and the computations will be carried out with respect to the *tdeg* term-ordering that is called *DegRevLex* in CoCoA. The line

```
Use T:=Z/(2)[x[1..2]z], DegRevLex;
```

gives the polynomials with coefficients 0,1 and in the indeterminates $x[1], x[2]$ and

z. Parameters are not allowed in CoCoA yet.

A polynomial ideal is defined by the function `Ideal`. For example the line
`FullFactorial:=Ideal(x^2 - 1, y^2 - 1, z^2 - 1);`
 defines the ideal generated by $x^2 - 1, y^2 - 1, z^2 - 1$. The Gröbner basis of an ideal I with respect to the term-ordering specified in the last line of the CoCoA section starting `Use`, is computed by the command `GBasis(I)`. Notice that the first letter of all commands in CoCoA is capital.

The remainder or normal form of a polynomial F with respect to an ideal I is returned by the command `NF(F, I)`. Differently from the *normalf* command in Maple, `NF` checks if the polynomials given to define I form a Gröbner basis and if not it computes it.

The function `Elim(t, I)` eliminates the variable t from the ideal I .

There is no a specific function to factorise polynomials but there are many other useful functions such as `Support(F)` that returns the list of terms of F and `LogToTerm(L)` that returns the terms whose list of exponents is L .

Appendix .2 includes the CoCoA code of the Buchberger algorithm for complex numbers and some examples. This is not a version of cocoa with complex numbers, but only a set of procedures that allow us to deal with complex numbers up to the computation of the Gröbner basis.

.2 Buchberger algorithm for complex numbers

The following is a high level CoCoAL version of the Buchberger algorithm, with some modifications that allow to deal with complex $(k[t]/(t^2 + 1))$ numbers. Ad hoc modifications allow to adapt the code for other extension fields. The main procedure, Buch, compute the Gröbner basis of an ideal over the complex field. Some other procedures implement the usual operation over the complex field. This is not a version of CoCoA with complex numbers but only a set of procedures that allow to deal with complex numbers up to the computation of the Gröbner basis. Every operation depending on Gröbner bases is interpreted by the system as an operation over the ring, not as an operation over the quotient ring. Only the operation showed below give results in the quotient ring.

Examples of the application of the code follow.

```
-- Complex Numbers Procedures

IIndet:=Indet(NumIndets()); -- The indeterminate i

Define CProduct(...)
  Resu:=1;
  For I:=1 To Len(ARGV) Do
    Resu:=Resu*ARGV[I];
  End;
  Return NF(Resu,[IIndet^2+1]);
End;

St(Z):=NF(Z,[IIndet^2+1]); -- Canonical representant of Z

Im(Z):=CoeffOfTerm(IIndet,Z);
Re(Z):=CoeffOfTerm(1,Z);
NormQ(Z):=CoeffOfTerm(1,Z)^2+CoeffOfTerm(IIndet,Z)^2;
Inv(Z):=(Re(Z)-IIndet*Im(Z))/NormQ(Z);

Define C_Log(T);
  L:=Log(T);
  L[NumIndets()]:=0;
  Return L;
End;

Define C_LT(P) -- Leading Term
  L:=C_Log(LT(P));
  Return LogToTerm(L);
End;

Define C_LC(P) -- Leading Coefficient
  If Der(LT(P),IIndet)=0
  Then Return Cast(LC(P),POLY) -- guarda il tipo di quello sotto
```



```

Else
  If C_LT(P-LT(P)*LC(P))=C_LT(P)
  Then Return Cast((LC(P)*LT(P))/C_LT(P)+LC(P-LT(P)*LC(P)),POLY)
  Else Return Cast((LC(P)*LT(P))/C_LT(P),POLY)
  End;
End;
End;

C_LM(P):=C_LT(P)*C_LC(P); -- Leading Monomial
IsC_Const(Z):=Z=C_LC(Z); -- Is Z a constant?

Define TermDivides(S,T)
  L1 := C_Log(S);
  L2 := C_Log(T);
  For I := 1 To NumIndets Do
    If L1[I]>L2[I] Then Return False End
  End;
  Return True;
End;

Define TermsAreCoprime(S,T)
  L1 := C_Log(S);
  L2 := C_Log(T);
  For I := 1 To NumIndets Do
    If L1[I]*L2[I] <> 0 Then Return False End
  End;
  Return True;
End;

Define TermLCM(S,T)
  L1 := C_Log(S);
  L2 := C_Log(T);
  Return LogToTerm([Max(L1[I],L2[I]) | I In 1..NumIndets]);
End;

Define TermLT_AntiDegRevLex(S,T)
  If Deg(S) < Deg(T) Then Return True End;
  If Deg(S) > Deg(T) Then Return False End;
  L1 := Log(S); L2 := Log(T);
  For K := NumIndets To 2 Step -1 Do
    If L1[K] < L2[K] Then Return False End;
    If L1[K] > L2[K] Then Return True End;
  End;
  Return False
End;

--- Complex Normal Form

```

```

Define C_FindReductor(LTM,Lista, Var Found)
  N:=Len(Lista);
  Found:=0;
  I:=1;
  While I<= N Do
    If Mod (LTM,C_LT(Lista[I]))=0
      Then
        Found:=Lista[I];
        Return Null
      End;
    I:=I+1;
  End;
  Return Null
End;

```

```

Define C_NormalForm(P,B)
  Irred:=0;
  Found:=0;
  While P<>0 Do
    C_FindReductor(C_LT(P),B,Found);
    If Found<>0 Then
      P:= P-St(Found*C_LM(P)*Inv(C_LC(Found))/C_LT(Found));
    Else
      Irred:=Irred+C_LM(P); -- aggiunge la testa a irred
      P:=P-C_LM(P); --taglia la testa
    End;
  End;
  Return Irred;
End;

```

```

Define C_Interreduced(L)
  I:=1;
  While I<=Len(L) Do
    L[I]:=C_NormalForm(L[I],Concat(First(L,I-1),Last(L,Len(L)-I)));
    If L[I]=0 Then
      L:=Concat(First(L,I-1),Last(L,Len(L)-I));
    Else
      I:=I+1;
    End;
  End;
  Return L;
End;

```

---- Procedures for the Buchberger algorithm

-- Pairs management

```
PairsLT(P1,P2) := TermLT_AntiDegRevLex(P1[3],P2[3]);
```

```
PairsGT(P1,P2) := PairsLT(P2,P1);
```

```
Define BuildNewPair1(P)
  Return [P,0,C_LT(P),FALSE]
End;
```

```
Define BuildNewPair(F,G)
  P := NewList(4);
  P[1] := F;
  P[2] := G;
  P[3] := TermLCM(C_LT(F),C_LT(G));
  P[4] := TermsAreCoprime(C_LT(F),C_LT(G));
  Return P
End;
```

```
Define FirstPairGT(Var Pairs,P)
  For I := 1 To Len(Pairs) Do
    If PairsGT(Pairs[I],P) Then Return I End
  End;
  Return 0
End;
```

```
Define InsertPair(Var Pairs,P) Append(Pairs,P) End;
MergePairs(Ps1,Ps2) := Concat(Ps1,Ps2);
OnlyNotCoprimes(L) := [ P In L | Not P[4] ];
```

```
Define InsertPairGM(Var Pairs,P)
  L := P[3];
  I := 1; N := Len(Pairs);
  ToBeInserted := True;
  While I<=N And ToBeInserted Do
    LI := Pairs[I][3];
    If L=LI Then
      If Pairs[I][4] Or Not P[4] Then ToBeInserted := False
      Else Pairs[I] := P; ToBeInserted := False
    End
  Else
    If TermDivides(L,LI) Then Pairs[I] := Null
    Else
      If TermDivides(LI,L) Then ToBeInserted := False End;
    End
  End;
  I := I + 1
End;
```

```

Pairs := [ P In Pairs | Type(P) <> NULL ];
If ToBeInserted Then InsertPair(Pairs,P) End
End;

```

```

Define BCriterion(Var Pairs, T)
  N := Len(Pairs);
  Pairs := [P In Pairs | Not (TermDivides(T,P[3])
                             And TermLCM(T,C_LT(P[1])) <> P[3]
                             And TermLCM(T,C_LT(P[2])) <> P[3]) ];
End;

```

```

Define BuildNewPairs(Var GB,F)
  N := Len(GB);
  Pairs := [];
  For I := 1 To Len(GB) Do
    P := BuildNewPair(GB[I],F);
    If C_LT(GB[I]) = P[3] Then
      GB[I] := Null
    End;
    InsertPairGM(Pairs,P)
  End;
  M := Len(GB);
  GB := [F In GB | Type(F) <> NULL ];
  FPairs := OnlyNotCoprimes(Pairs);
  Return FPairs
End;

```

```

Define UpdateBasisAndPairs(Var GB, Var R, Var Pairs, F)
  BCriterion(Pairs,F);
  NewPairs := BuildNewPairs(GB,F);
  InsertReductor(F,R);
  Append(GB,F);
  Pairs := MergePairs(Pairs,NewPairs);
End;

```

-- Reductors management

```

ReductorLT(P1,P2) := TermLT_AntiDegRevLex(P1,P2);
ReductorGT(P1,P2) := ReductorLT(P2,P1);

```

```

Define ReductorFirstGT(Var L, P)
  For I := 1 To Len(L) Do
    If ReductorGT(L[I],P) Then Return I End
  End;
  Return 0
End;

```

```

Define InsertReductor(P,Var L)
  Append(L,P)
End;

--- S-Polynomial management

SPoly1(P):=P[1];

Define SPoly2(P)
  F := P[1];
  G := P[2];
  A := P[3];
  Return
    St(C_LC(G)*(A/C_LT(F))*Inv(C_LC(F))*
      F - C_LC(F)*(A/C_LT(G))*Inv(C_LC(G))*G)
End;

Define SPoly(P);
  If P[2]=0
  Then Return SPoly1(P)
  Else Return SPoly2(P)
  End;
End;

-- Miscellanea

Monic(L) := [St(X*Inv(C_LC(X))|X In L];
NormalForm(P,L) := NF(P,L);

--- Main algorithm

Define Buch(L)
  If Len(L) <= 1 Then Return L End;
  NoUsefulSP:= 0;
  NoUselessSP:=0;
  GB := [Head(L)];
  R := [Head(L)];
  Pairs := [];
  InsertPair(Pairs,BuildNewPair1(Head(L)));
  Foreach P In Tail(L) Do
    InsertPair(Pairs,BuildNewPair1(P));
  End;
  While Pairs <> [] Do
    SP := SPoly(Head(Pairs));
    Pairs := Tail(Pairs);
    SP := C_NormalForm(SP,R);
  End;

```

```
If SP <> 0 Then
  UpdateBasisAndPairs(GB,R,Pairs,SP);
  NoUsefulSP:=NoUsefulSP+1;
Else
  NoUselessSP:=NoUselessSP+1;
End;
End;
Return Monic(C_Interreduced(GB));
End;
```

```

Use S:=Q[x,y,z,i],Ord( 1,1,1,0,
                        0,0,-1,0,
                        0,-1,0,0,
                        0,0,0,1);

-- the ring Q(i)[x,y,z];
Im(3i+2);
3

Re(3i+2);
2

Inv(i+1);
- 1/2i + 1/2

-- The square of the norm
NormQ(1+i);
2

NormQ(2+3i);
13

-- Product of polys over S
CProd(i+1,x+i,xi-y);
x^2i - x^2 - xyi - xy - xi - x - yi + y

-- Put a poly over S in normal form
St(i^4x+xyi^3+i+1);
- xyi + x + i + 1

-- The log of a term
C_Log(xy^2i^3);
[1, 2, 0, 0]

-- The leading term of a poly
C_LT(xyi+xy+yi^4);
xy

-- The leading coefficient of a poly
C_LC((xyi+xy+yi^4));
i + 1

-- The computation of a Gbasis over S
I:=Ideal( x^2yi^3 + 2x^2y - z^3,

```

$y^3i - z^3$);

C_GBasis(I);

[$x^2y - 1/5z^3i - 2/5z^3$,
 $y^3 + z^3i$,
 $x^2z^3 - 2/5y^2z^3i + 1/5y^2z^3$]

-- Normal Form Computations

L:= [$x^2y - 1/5z^3i - 2/5z^3$,
 $y^3 + z^3i$,
 $x^2z^3 - 2/5y^2z^3i + 1/5y^2z^3$];
C_NormalForm($x^2yi^3+xyz+i$,L);
 $xyz - 2/5z^3i + 1/5z^3 + i$

"E quindi uscimmo a riveder le stelle."

Dante, Inferno, XXXIV-139