Abstract: Identifiability of polynomial models is a key requirement for multiple regression. We consider an analogue of the so-called statistical fan, the set of all maximal identifiable hierarchical models, for cases of noisy experimental designs or measured covariate vectors with a given tolerance vector. This gives rise to the definition of the numerical statistical fan. It includes all maximal hierarchical models that avoid approximate linear dependence of the model terms. We develop an algorithm to compute the numerical statistical fan using recent results on the computation of all border bases of a design ideal from the field of algebra. The ideas are applied to data from a thermal spraying process. It turns out that the numerical statistical fan is effectively computable and much smaller than the respective statistical fan. The gained enhanced knowledge of the space of all stable identifiable hierarchical models enables improved model selection procedures.

Key words and phrases: Algebraic statistics, identifiable regression models, hierarchical models, noisy experimental design, statistical fan.

1 Introduction

Model selection procedures play an integral part in regression analysis, with hierarchical polynomial models often being the maximal models. For many experimental designs like full factorial designs or central composite designs, the set of identifiable hierarchical maximal models is well-known and usually quite small as these designs exhibit many symmetries. However, we might not have an experimental setup with a well-established experimental design. Then, the set of all identifiable maximal hierarchical models is given by the statistical fan from the field of algebraic statistics (Pistone, Riccomagno and Wynn, 2000). A selection and search algorithm in the set of hierarchical models is suggested in
Bates, Giglio and Wynn (2003). If we are modeling some response $Y$ from a design $D_X$ given by a set of input data points $x_1, \ldots, x_n$, then - for generic input data - the statistical fan is hard to enumerate, because its size grows (sub)-exponentially with the number of data points. If the input data points are observed or measured, they come with errors. Given a tolerance vector that bounds these errors, we may define sets of points of limited precision or noisy designs. This gives rise to the question which hierarchical models are identifiable for such empirical designs. Our goal is to formalize and exploit the notion of a numerical statistical fans, which includes all maximal hierarchical models that avoid any kind of “numerical aliasing” between the model terms, i.e. any approximate linear dependence of the design vectors.

A subset of a numerical statistical fan, the numerical algebraic fan, has been previously introduced in [Rudak, Kuhnt and Riccomagno (2016)]. It is the numerical analogue of the algebraic fan which contains only hierarchical models that can be obtained by Gröbner basis techniques and which is usually only a small part of the desired statistical fan [Maruri-Aguilar, 2007].

In this contribution, we derive a recursive algorithm that effectively computes the numerical statistical fan, if the norm of the tolerance is not too small. Our algorithm is a modification of an algorithm proposed in [Hashemi, Kreuzer and Pourkhajouei (2019)] that computes all border bases (of a design ideal) and their order ideals. Actually, the first algorithm that allows to compute all border bases is given by [Braun, Pokutta, 2016]. They provided a polyhedral characterisation of identifiable order ideals which are in one-to-one correspondence to integral points of the so-called order ideal polytope.

We apply our methods to real data coming from thermal spraying. There we have a composite setting, i.e. generic design $D_Y$ that is itself the response to a well chosen experimental design $D_X$.

Section 2 introduces basic notions in algebraic statistics like order ideals, the statistical fan, Gröbner bases and the algebraic fan. Section 3 defines empirical designs, the notion of numerical linear dependence, stable order ideals and the numerical statistical fan of a noisy design. There we also describe the recursive algorithm to compute the numerical statistical fan. Section 4 deals with an application to thermal spraying data. We compute the numerical statistical fan, its size distribution of stable order ideals and we compare it to the statistical fan. Section 5 contains discussion and outlook.
2 Basic notions in algebraic statistics

In this section we introduce basic notion of algebraic statistics. In particular, Section 2.1 reveals design ideals, hierarchical models, design matrices and the statistical fan. Section 2.2 deals with Gröbner bases and the algebraic fan.

2.1 Hierarchical models and the statistical fan

A typical situation in applications of statistical design of experiments is that $d$ controllable input factors $X = (X_1, \ldots, X_d)^t$ influence a response $Y$. We run an experimental design $D$ with settings for $X$, observe response values $\{y(x)\}_{x \in D}$, and fit a linear regression model.

In algebraic statistics a design $D$ is viewed as the common zero set of polynomials in a so-called design ideal.

**Definition 1.** Let $R = K[X_1, \ldots, X_d]$ be the multivariate polynomial ring in $d$ variables $X_1, \ldots, X_d$ over the field $K$ (with $K = \mathbb{Q}$ or $\mathbb{R}$). A design $D = \{p_1, \ldots, p_n\}, n \in \mathbb{N}$, is a finite set of points in $K^d$. The design ideal $I(D)$ is the set of all polynomials in $R$ that vanish at the design points.

The set of all terms in $R$ is denoted by $T = \{X_1^{\alpha_1} \cdots X_d^{\alpha_d} | \alpha_i \geq 0, \ i = 1, \ldots, d\}$. This set is in one-to-one correspondence to $\mathbb{N}^d$ via some discrete logarithm map

$$\log : \ X^\alpha = X_1^{\alpha_1} \cdots X_d^{\alpha_d} \mapsto \alpha = (\alpha_1, \ldots, \alpha_d).$$

In general we are fitting polynomial models of the form $\sum_{\alpha \in S} \beta_\alpha X^\alpha$ with $S \subseteq \mathbb{N}^d$. Thus a polynomial model can be viewed as a finite set of terms and is completely described by the finite subset $S$ of $\mathbb{N}^d$. Of particular importance are hierarchical polynomial models, i.e. for any higher order term, the model also contains all of the lower order terms that compose it, e.g. with an interaction $X_1X_2$ also 1, $X_1$ and $X_2$ are contained in the model.

**Definition 2.** A hierarchical model or order ideal is a finite subset $O$ of $T$ that is closed under divisibility, i.e. $t \in O$ implies $t' \in O$ for all $t' | t$.

Note that $X^\alpha$ divides $X^\gamma$ if and only if $X_i^{\alpha_i}$ divides $X_i^{\gamma_i}$ for all $1 \leq i \leq d$. Hence divisibility of terms is mapped to the natural partial order on $\mathbb{N}^d$ via the above mentioned discrete logarithm. The subset $\log O \subseteq \mathbb{N}^d$ corresponding to an order ideal $O$ is also known as a staircase or, for $d = 2$, as Ferrers diagram or Young diagram. They are in one-to-one correspondence to (integer) partitions.

Similarly, hierarchical models in $d = 3$ dimensions correspond to so-called plane partitions. Generating functions for partitions and plane partitions are known due to Euler.
and MacMahon (1912), respectively. No such functions are known for \( d \geq 4 \) (Onn and Sturmfels, 1999).

Nevertheless, asymptotic results are known. Denote by \( p_d(n) \) the number of order ideals with \( n \) terms in \( d \) dimensions. Then, we have asymptotically \( p_d(n) = \Theta(\exp(n^{d-1/d})) \), i.e. the number of hierarchical models grows sub-exponentially (Bhatia, Prasad and Arora, 1997). Recall that the Big Theta notation \( f(n) = \Theta(g(n)) \) means that the function \( f \) is bound from above and below by \( g \) asymptotically. However, for \( n \) fixed, \( p_d(n) \) is polynomial in \( d \) of degree \( n - 1 \) (Atkin et al., 1967).

**Definition 3.** A term \( t = X^\alpha \) evaluated at \( D \) gives a design vector \( t(D) = (t(p_1), \ldots, t(p_n))^T \). These design vectors form the columns of the design matrix \( X_{\mathcal{O}}(D) := (X^\alpha(p))_{p \in D, \alpha \in \log \mathcal{O}} \).

Note that the design matrix depends on the model \( \mathcal{O} \) and the design \( D \), and it is only defined up to a permutation of the terms in \( \mathcal{O} \).

**Example 1.** Consider the 2-dimensional design \( D = \{(1, -1), (-1, 1), (-1, -1), (0, 0)\} \). The design vector of e.g. the term \( t = X^{(1,1)} = X_1X_2 \) (interaction between \( X_1 \) and \( X_2 \)) is \( t(D) = (-1, -1, 1, 0)^T \). The design matrix for the hierarchical model \( \mathcal{O} = \{1, X_1, X_2, X_1X_2\} \) is

\[
X_{\mathcal{O}}(D) = \begin{pmatrix}
1 & X_1 & X_2 & X_1X_2 \\
1 & 1 & -1 & -1 \\
1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 \\
1 & 0 & 0 & 0
\end{pmatrix}.
\]

The respective regression model would be described by

\[
E(Y|X) = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1X_2
\]

where \( \beta \) in \( \mathbb{R}^4 \) is the unknown parameter vector to be estimated by the least squares method.

In fitting regression models the problem of non-identifiability occurs if least-squares-estimates are not unique. We next provide an algebraic definition for the set of identifiable models with respect to a given design.

**Definition 4.** A model is identifiable if the design matrix \( X_{\mathcal{O}}(D) \) is of full rank. The statistical fan \( S(D) \) of a design is the set of hierarchical models identifiable by the design with as many terms as distinct design points. In other words, it is the set of all maximal identifiable order ideals.
**Example 2.** Consider again the 2-dimensional design $D = \{(1, -1), (-1, 1), (-1, -1), (0, 0)\}$. Its statistical fan $S(D)$ contains three models, namely $\mathcal{O}_3 = \{1, X_1, X_2, X_1X_2\}$, $\mathcal{O}_2 = \{1, X_1, X_2, X_1^2\}$, and $\mathcal{O}_3 = \{1, X_1, X_2, X_2^2\}$. Figure 1 displays the Ferrers diagrams of the order ideals $\mathcal{O}_1, \ldots, \mathcal{O}_3$. The marked points all lie in the lattice $\mathbb{N}^2 \subset \mathbb{R}^2$ and they represent exponents, i.e., discrete logarithms, of bivariate terms, e.g., $(2, 0)$ stands for $X^{(2, 0)} = X^2_1$. The lattice points on the abscissa represent powers of $X_1$ and the lattice points on the ordinate powers of $X_2$.

![Ferrers diagrams](image)

**Figure 1:** Ferrers diagrams of the order ideals $\mathcal{O}_1, \ldots, \mathcal{O}_3$ with the associated monomials.

For a generic design $D$ with $|D| = n$, all models (with $n$ terms) are identifiable [Pistone, Riccomagno and Wynn 2000]. Hence, the size of the statistical fan is bounded sub-exponentially in $n$.

### 2.2 Gröbner bases and algebraic fan

Let $\prec$ be a *term order* on $\mathcal{T}$, i.e., a total ordering on $\mathcal{T}$ which is multiplicative and a well-ordering. For a non-zero polynomial $f \in R$, we denote by $\text{LT}(f)$ its *leading term*, that is the greatest term occurring in $f$ with respect to $\prec$. For an ideal $I$ in $R$, let $\text{LT}(I)$ be the ideal generated by all $\text{LT}(f)$ with $f \in I$, formally $\text{LT}(I) := \langle \text{LT}(f) \mid f \in I \rangle$.

**Definition 5.** A finite generating subset $G \subseteq I$ is called a *Gröbner basis* for $I$ w.r.t. $\prec$ if $\text{LT}(I) = \langle \text{LT}(g) \mid g \in G \rangle$. We use the notation $G = G_\prec(I)$.

The set of all terms that are not divided by the leading terms of the Gröbner basis $G = G_\prec(I)$ form an hierarchical model $\mathcal{O}$. The residue classes of these terms in $\mathcal{O}$ form a vector space basis of the quotient ring $R/I$. We call $(\mathcal{O}, G)$ a *Gröbner pair* for the ideal $I$.

**Example 3.** Consider the $2^2$-factorial design $D = \{(1, -1), (-1, 1), (-1, -1), (1, 1)\}$. Since the values of the $X_1$- and $X_2$-coordinate are restricted to $\pm 1$, we know that the vanishing ideal $I = I(D)$ is generated by $X_1^2 - 1 = (X_1 - 1)(X_1 + 1)$ and $X_2^2 - 1$. Indeed, these two
polynomials form the Gröbner basis $G$ of $I$ for any term ordering $\prec$. The terms not divided by the leading terms $X_1^2$ and $X_2^2$ form the hierarchical model $O = \{1, X_1, X_2, X_1X_2\}$.

We next provide a definition of the set $A(D)$ of all maximal identifiable hierarchical models that can be obtained using Gröbner basis techniques.

**Definition 6.** The algebraic fan $A(D)$ of a design $D$ is the set of all hierarchical models $O$ such that $(O, G_{\prec}(I))$ is a Gröbner pair for the design ideal $I = I(D)$ if we run through all term orders $\prec$.

The algebraic fan $A(D)$ is a subset of the statistical fan $S(D)$ and is in general much smaller than the latter. $A(D)$ cannot contain more elements than there are reduced Gröbner bases for $I$. The number of distinct reduced Gröbner bases is connected to so-called corner cuts (Onn and Sturmfels, 1999) and is asymptotically of order $O(n^{2d(d-1)/d+1})$. Hence the size of $A(D)$ grows polynomially in $n = |D|$ for fixed dimension $d$.

### 3 Numerical statistical fan

Measurements come with errors - so do “design” points that are results from measurements themselves. We are interested in identifiable maximal models that do not depend on small perturbations of the design points. Such “stable” models will also exhibit numerical stability.

A measure of instability of a system of linear equations $Ax = b$ is the **condition number** $c(A) := ||A|| \cdot ||A^{inv}||$ where $A^{inv}$ is the Moore-Penrose pseudoinverse of $A$ and $||\cdot||$ indicates some matrix norm. We will use only the induced 2-norm as matrix norm. The condition number of a square matrix is always at least 1. If it is much larger than 1 then the matrix is ill-conditioned.

**Example 4.** (Rudak, Kuhnt and Riccomagno, 2016) Consider the design $D = \{(1, 1), (1, -1.001), (-1, 1), (-1, -1)\}$. Its algebraic and statistical fan are identical, and $S(D)$ has two identifiable models, namely $O_1 = \{1, X_1, X_2, X_1X_2\}$ and $O_2 = \{1, X_1, X_2, X_2^2\}$ with corresponding design matrices

$$X_{O_1}(D) = \begin{pmatrix} 1 & X_1 & X_2 & X_1X_2 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & -1.001 & -1.001 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \quad X_{O_2}(D) = \begin{pmatrix} 1 & X_1 & X_2 & X_2^2 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & -1.001 & 1.002001 \\ 1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 \end{pmatrix}.$$
For $X_{O_1}(D)$ we get almost $c(X_{O_1}(D)) = 1.0007$ and for $X_{O_2}(D)$ we have $c(X_{O_2}(D)) = 4001$. Indeed, the design vectors $t_1(D) = (1, 1, 1, 1)^t$ and $t_2(D) = (1, 1.002001, 1, 1)^t$ (for $t_1 = 1$ and $t_2 = X_2^2$) are very close to each other. That can be explained by the fact that there is a close perturbed design $\tilde{D}$, namely the $2^2$ full factorial design $\{(\pm 1, \pm 1)\}$ for which $t_1(\tilde{D})$ and $t_2(\tilde{D})$ coincide. Indeed, $S(\tilde{D})$ has only one leaf $O_1 = \{1, X_1, X_2, X_1X_2\}$.

More generally, we need to define numerical linear dependence for design vectors with error. Several notions of numerical linear dependence have been suggested. Since linear dependence of design vectors is connected to polynomials vanishing at the design, one approach is to bound the evaluation of normed polynomials by a real threshold parameter $\epsilon > 0$. This is done e.g. in Heldt et al. (2009) and Limbeck (2014). We follow another approach that requires the knowledge of the tolerance on the data uncertainty, i.e. a tolerance vector (Stetter, 2004; Abbott, Fassino and Torrente, 2008; Fassino, 2010; Torrente, 2009).

3.1 Numerical dependence of empirical points

We need a proper definition of perturbations in order to capture the notion of a noisy design with errors.

**Definition 7.** Let $p = (c_1, \ldots, c_d)$ be a point in $\mathbb{R}^d$ and let $\delta = (\delta_1, \ldots, \delta_d)$ with $\delta_i \geq 0$ be a given vector of componentwise tolerances. A point $\tilde{p} \in \mathbb{R}^d$ is an $\delta$-perturbation of $p$ if $|\tilde{c}_i - c_i| < \delta_i$ for all $i = 1, \ldots, d$.

Let $D$ be a given design. A pair $(D, \delta)$ is called an empirical design. A design $\tilde{D}$ is a $\delta$-perturbation of the design $D$ if a one-to-one mapping between $D$ and $\tilde{D}$ exists, such that each point $\tilde{p} \in \tilde{D}$ is a $\delta$-perturbation of the corresponding point $p \in D$.

We will also call an empirical design a noisy design or a set of points of limited precision.

Next we define numerical linear dependence of empirical design vectors through the existence of a perturbed design for which we have exact linear dependence.

**Definition 8.** Given a set $O = \{t_1, \ldots, t_k\}$, an empirical design $(D, \delta)$, and a monomial $t$, the design vector $t(D)$ numerically depends on $\{t_1(D), \ldots, t_k(D)\}$ if there exists a $\delta$-perturbation $\tilde{D}$ of $D$ such that the residual $\rho(\tilde{D})$ of the least squares problem $X_O(\tilde{D})\tilde{a} \approx t(\tilde{D})$ is a zero vector.

We only know the evaluations at the design $D$, and we can only solve the least squares problem $X_O(D)a \approx t(D)$ for $a$. Nevertheless, Proposition 1 allows us to infer results for a
perturbed design $\hat{D}$.

**Proposition 1.** (Fassino, 2010) If there exists a $\delta$-perturbation $\hat{D}$ of $D$ such that $\rho(\hat{D}) = 0$ for the residual of the least squares problem $X_\mathcal{O}(\hat{D})\hat{a} \approx t(\hat{D})$, then the residual vector $\rho(D)$ (of the least squares problem $X_\mathcal{O}(D)a \approx t(D)$) satisfies

$$|\rho(D)| \leq |I - X_\mathcal{O}(D)X_\mathcal{O}^{\text{inv}}(D)| \sum_{k=1}^{d} \delta_k |\partial_k t(D) - X_{\partial_k \mathcal{O}}(D)a| + O(\delta_M^2)$$

(1)

Here $\delta_M = \max_{i=1}^{d} \delta_i$ and $X_\mathcal{O}^{\text{inv}}(D)$ is the Moore-Penrose inverse of the design matrix, i.e. $X_\mathcal{O}^{\text{inv}}(D) = (X_\mathcal{O}^t(D)X_\mathcal{O}(D))^{-1}X_\mathcal{O}^t(D)$. And $\partial_k t$ denotes the partial derivative of the term $t$ with respect to $X_k$. Hence, $\partial_k t$ is in general not a term since it is not necessarily normed (i.e. the coefficient may be $\neq 1$). Similarly, $\partial_k \mathcal{O}$ denotes the multiset of all $\partial t/\partial X_k$ for $t$ in $\mathcal{O}$. Hence, $X_{\partial_k \mathcal{O}}(D)$ is the matrix $(\partial_k t(p))_{p \in D, t \in \mathcal{O}}$.

Inequality (1) provides a sufficient condition for showing that $t(D)$ is numerically independent of the columns of $X_\mathcal{O}(D)$. If we drop the $O(\delta_M^2)$ term, the Fassino condition becomes a heuristical condition for numerical independence.

More precisely, given a set $\mathcal{O} = \{t_1, \ldots, t_k\}$, an empirical design $(D, \delta)$, and a monomial $t$, the design vector $t(D)$ is declared to be numerically independent of $\{t_1(D), \ldots, t_k(D)\}$ if the residual $\rho(D)$ (of the least squares problem $X_\mathcal{O}(D)a \approx t(D)$) satisfies

$$|\rho(D)| > \sum_{j=1}^{n} |I - X_\mathcal{O}(D)X_\mathcal{O}^{\text{inv}}(D)|_{ij} \sum_{k=1}^{d} \delta_k |\partial_k t(D) - \sum_{l=1}^{|\mathcal{O}|} X_{\partial_k \mathcal{O}}(D)_{jl} a_l|$$

(2)

for one design point $p_i \in D$. To prove numerical dependence it would be preferable to find a $\delta$-perturbation $\hat{D}$ of $D$ such that $\rho(\hat{D}) = 0$. This is done in the root finding algorithm of Fassino and Torrente (2013). In the applications in Section 4 we only deploy the heuristical Fassino condition (2) which we use as a proxy for numerical dependence. Recall that, even if the $O(\delta_M^2)$ term is negligible, then condition (2) is only a sufficient condition for numerical independence. Hence, by checking condition (2), we might declare numerical dependence when there is none, i.e. the residuals are all small, but there exists no $\delta$-perturbed design on which they vanish exactly. We regard this as a good property of the heuristical Fassino condition (2), because such numerically independent terms which are close to dependence (in the sense that the residuals are small) may lead to bad (high) condition numbers. By deploying condition (2) we guarantee that the norm of the residual vector is above some lower bound. This leads to a flexible upper bound for the evaluation of polynomials (divided by some polynomial norm) which describe linear dependencies between design vectors. In this sense our approach incorporates the idea of a real threshold.
parameter $\epsilon > 0$ for normed almost vanishing polynomials as in Heldt et al. (2009); Limbeck (2014), but we do not have a fixed $\epsilon > 0$ which has to be fine-tuned. In our case it depends on the model $\mathcal{O}$ and the empirical design $(D, \delta)$. In particular, we use knowledge about the tolerance on the data uncertainty given by the vector $\delta$.

### 3.2 Stable order ideals and numerical fans

The following definition captures an analogue of the notion of identifiability (of a model) in the context of noisy designs.

**Definition 9.** Let $(D, \delta)$ be an empirical design. An order ideal $\mathcal{O}$ is called *numerically stable* (or just *stable*) if the evaluation matrix $X_{\mathcal{O}}(\tilde{D})$ has full rank for each $\delta$-perturbation $\tilde{D}$ of $D$.

Note that the design (or evaluation) vectors of all monomials in a numerically stable order ideal $\mathcal{O}$ are numerically independent. The notion of stable order ideals allows us to introduce a numerical analogue of the statistical fan of a design.

**Definition 10.** The set of all maximal (w.r.t. inclusion) stable order ideals of an empirical design $(D, \delta)$ is called the *numerical statistical fan* $S_{\text{num}}(D, \delta)$ of the empirical design.

In the next subsection we will tackle the problem of computing the numerical statistical fan of an empirical design. First we describe a strategy to find some/any stable order ideal. Note that an order ideal $\mathcal{O}$ can be efficiently encoded by its maximal elements (w.r.t. divisibility) or equivalently by the minimal elements of its complement $T - \mathcal{O}$. These minimal elements form the *corner set* of $\mathcal{O}$. They are precisely the monomials $t$ such that $\mathcal{O} \cup \{t\}$ is again an order ideal. Therefore they are the new candidate elements to be included in $\mathcal{O}$ in a recursive computation of $\mathcal{O}$. This recursive computation of a stable order ideal $\mathcal{O}$ is a modification of the Möller-Buchberger (also called Buchberger-Möller) algorithm (Möller and Buchberger 1982). By $J$ we denote the *monomial ideal* generated by the corners of $\mathcal{O}$.

1. Initialize $\mathcal{O} = \{1\}$ and $J = (0)$.

2. Choose a term $t$ in the corner set of $\mathcal{O}$ not belonging to $J$. If no such $t$ exists, return $\mathcal{O}$ and stop.

3. If $t(D)$ is numerically linear independent of $\mathcal{O}(D)$ then add $t$ to $\mathcal{O}$. Otherwise, add $t$ to the set of generators of $J$.
4. Go to step 2.

Note that any strategy that chooses a candidate term \( t \) in the corner set of \( \mathcal{O} \) can be applied. In the Möller-Buchberger algorithm \cite{MollerBuchberger1982} - as well as its numerical analogue, the numerical Buchberger-Möller (NBM) algorithm \cite{Fassino2010} - the monomial \( t \) is chosen as the smallest candidate w.r.t. a fixed monomial ordering \( \prec \). Indeed, given an empirical design \((D, \delta)\) and a term ordering \( \prec \), the NBM algorithm returns a stable order ideal \( \mathcal{O} \) and a set \( G \) of of almost vanishing polynomials on \( D \). The output \((\mathcal{O}, G)\) from the NBM algorithm is the numerical analogue to the Gröbner pair provided by the classical Möller-Buchberger algorithm. Given a tolerance vector \( \delta \), numerical linear dependence is checked in the NBM algorithm \cite{Fassino2010} by the heuristic Fassino condition.

**Definition 11.** \cite{RudakKuhntRiccomagno2016} Let \((D, \delta)\) be an empirical design. The numerical algebraic fan \( A_{\text{num}}(D, \delta) \) is the set of all stable order ideals \( \mathcal{O} = \mathcal{O}_{\prec} \) such that \((\mathcal{O}_{\prec}, G_{\prec})\) is the output of an NBM algorithm, running through all term orderings \( \prec \).

By definition, the numerical algebraic fan \( A_{\text{num}}(D, \delta) \) is a subset of the numerical statistical fan \( S_{\text{num}}(D, \delta) \). Let \( \| \cdot \| \) be any vector norm. In the limit \( \| \delta \| \to 0 \), we get \( A_{\text{num}}(D, \delta) \to A_{\text{num}}(D) \) and \( S_{\text{num}}(D, \delta) \to S_{\text{num}}(D) \), respectively. More precisely, there exists a \( \delta_{\text{min}} > 0 \) such that for all \( \delta < \delta_{\text{min}} \) we have \( A_{\text{num}}(D, \delta) = A_{\text{num}}(D) \) and \( S_{\text{num}}(D, \delta) = S_{\text{num}}(D) \).

We are interested in the numerical statistical fan \( S_{\text{num}}(D, \delta) \) since it gives us all maximal stable order ideals. The numerical algebraic fan \( A_{\text{num}}(D, \delta) \) may be an important subset of \( S_{\text{num}}(D, \delta) \) to consider, if the numerical statistical fan is not feasible to compute. This is not the case in our applications.

Note that the computation of the numerical algebraic fan has not been implemented yet. In \cite{RudakKuhntRiccomagno2016} only a subset of \( A_{\text{num}}(D, \delta) \) is computed by choosing three popular term orderings and permuting the coordinates.

### 3.3 Computation of the statistical fan

Hashemi, Kreuzer and Pourkhajouei \cite{HashemiKreuzerPourkhajouei2019} suggest a recursive algorithm to compute all border bases of a finite 0-dimensional ideal \( I = I(D) \). This algorithm necessarily also computes all maximal order ideals and can thus be utilized to get the statistical fan \( S(D) \).

The following algorithms are modifications of Algorithms 3 and 4 from \cite{HashemiKreuzerPourkhajouei2019}. The function AllOrderIdeals() (see Algorithm 1) computes a
list $L$ of all maximal order ideals for a design $D$. It simply initializes an empty list $L$, an empty order ideal $O$ and its corresponding design matrix $M$, and calls the main function AllOIStep.

**Algorithm 1: AllOrderIdeals()**

1. Initialize $L := []$ (empty list);
2. Initialize $O = {}$;
3. Initialize $M$ as $n \times 0$-matrix;
4. $L, O, M := \text{AllOIstep}(L, O, M)$;

The main function AllOIStep($L, O, M$) (see Algorithm 2) changes the list $L$, the current order ideal $O$ and its corresponding design matrix $M = X_{O}(D)$. It adds to the list $L$ all maximal order ideals that contain the current order ideal $O$. An order ideal $O$ is added to the list if it has maximal size $n = |D|$ and was not added earlier. If $O$ is not maximal, we check for all terms $t$ in the corner set $S$ of $O$ whether the design vector $t(D)$ is linear independent of the columns of the design matrix $M$. In the case of linear independence the function calls itself to add all maximal order ideals that contain $O \cup \{t\}$. Since $O$ and $M$ are updated and we run through all $t \in S$, we have to store the original $O_{in} := O$ (and $M_{in} := M$) that has corner set $S$.

**Algorithm 2: AllOIStep($L, O, M$)**

1. $O_{in} := O;$ $M_{in} := M$;
2. if $|O| = n$ and $O \notin L$ then append $O$ to list $L$;
3. if $|O| < n$ then
   4. $S := \text{set of all terms } t \notin O \text{ s.t. } O \cup \{t\} \text{ is an order ideal.}$;
   5. for $t$ in $S$ do
      6. $O := O_{in};$ $M := M_{in}$;
      7. if $t(D)$ is linear independent of columns of $M$ then
          8. Add $t(D)$ as last column to $M$;
          9. $L, O, M := \text{AllOIstep}(L, O \cup \{t\}, M)$;
      end
   end
4. end

return $L, O, M$;

Note that in Hashemi, Kreuzer and Pourkrajouei (2019) the design vector $t(D)$ was
first reduced with respect to the columns of $M$ before it was added as a new column. Reduction is not wanted for finding the numerical statistical fan as the design vectors $t(D)$ (the columns of $M$) are itself of interest. Here, we want to find numerical linear dependencies between the original design vectors rather than reduced linear combinations of them.

### 3.4 Computation of the numerical statistical fan

In order to compute the numerical fan $S_{num}(D, \delta)$ we adapt Algorithm 2 by replacing linear independence by numerical linear independence. However, this is not sufficient. It is clear that Algorithms 1 and 2 cannot be used directly to compute the numerical statistical fan since the breaking condition in Algorithm 2 is $|O| = n$, but maximal stable order ideals might have $|O| < n$.

Numerical linear independence can be empirically checked by deploying the heuristical Fassino condition. Since this condition is not sufficient for numerical dependence, it might provide some false positives. In this context we distinguish two concepts of maximality of stable order ideals, namely weakly maximal and maximal.

**Definition 12.** Let $(D, \delta)$ be an empirical design. A stable order ideal $O$ is called *weakly maximal* if $t(D)$ is numerically dependent of $X_O(D)$ for all $t$ in the corner of $O$. A stable order ideal $O$ is called *maximal* if there exists no stable order ideal $O'$ such that $O \subset O'$. If $O$ is maximal, then it is weakly maximal. However, the opposite may not hold when we check numerical dependence by the heuristical Fassino condition. For example, the following situation might occur. For $t \neq t'$ and $t, t' \notin O$, let $O \cup \{t\}$ and $O \cup \{t'\}$ both be stable order ideals with $O \cup \{t\}$ also being weakly maximal. Hence, $t'$ numerically depends on $O \cup \{t\}$ according to the heuristic condition (2). However, $t$ may be numerically independent of $O \cup \{t'\}$, and thus will be included to provide the stable order ideal $O \cup \{t, t'\}$ proving $O \cup \{t\}$ to be weakly maximal, but not maximal. We see that such a situation occurs because the Fassino conditions (1) and (2) are not symmetrical in $\{t, t_1, \ldots, t_p\}$ for a model $O = \{t_1, \ldots, t_p\}$, i.e. we have a heuristic notion of $t(D)$ being numerically dependent of the columns of $X_O(D)$, but no symmetric heuristic notion of numerical dependence of $\{t(D), t_1(D), \ldots, t_p(D)\}$.

To deal with this problem we use the Fassino condition, but then eliminate all order ideals which are not maximal. Hence, Algorithm 3 first computes a list $L$ of all weakly maximal order ideals using as main function Algorithm 4. Then, in order to get the numerical statistical fan of maximal stable order ideals, one has to check for inclusions $O \subseteq O'$ in
the list $L$, and we keep only the maximal order ideals w.r.t. inclusion.

**Algorithm 3: AllStableOrderIdeals()**

1. Initialize $L := []$; $HL := []$ (empty lists);
2. Initialize $O := \{\}$;
3. Initialize $S := \{1\}$;
4. Initialize $M$ as $n \times 0$-matrix;
5. $L, O, S, M, HL := \text{AllStableOIstep}(L, O, S, M, HL)$;
6. for $O$ in $L$ do
   7.     for $O'$ in $L$ do
   8.         if $O \subsetneq O'$ then Remove $O$ from list $L$;
   9.     end
10. end
11. return $L$

Algorithm 4 is a function that calls itself in order to compute all weakly maximal stable order ideals that contain a given order ideal $O$.

Improving Algorithm 2, here we also update the corner set $S$ of $O$ and a list $HL$ of all visited order ideals. This has two benefits. First, it is much faster to compute the corner set of $O \cup \{t\}$ from $S$ - the corner set of $O$ - rather than from $O \cup \{t\}$. Second, by using a list of all order ideals, we avoid visiting an order ideal several times. Here we can replace the list $HL$ of order ideals by a list of corner sets for efficiency. Furthermore, it can be replaced by a hash list (therefore $HL$) of hash values, because we are not interested in all order ideals - only in the (weakly) maximal stable ones.

An order ideal is added to the list $L$ if $\text{Maxbool} == TRUE$, i.e. if for all $t \in S$, $t(D)$ is numerically linear dependent of the columns of $M$ according to condition (2). That is the definition of a weakly maximal stable order ideal.

### 3.5 Examples

In this subsection we apply the algorithms from Sections 3.3 and 3.4 to compute the statistical fan and the numerical statistical fan for some small examples of (empirical) designs.

**Example 5.** Consider again the design $D = \{(1, 1), (1, -1.001), (-1, 1), (-1, -1)\}$ from the beginning of Section 3. Its statistical fan $S(D)$ has two identifiable models, namely
Algorithm 4: AllStableOIStep($L, O, S, M, HL$)

1. $O_{in} := O; S_{in} := S; M_{in} := M$
2. if $O \notin L$ then
   3. Maxbool := TRUE;
   4. for $t$ in $S_{in}$ do
      5. $O := O_{in}; S := S_{in}; M := M_{in}$;
      6. if $t(D)$ is num. linear independent of columns of $M$ then
         7. Maxbool := FALSE;
      8. if $O \notin HL$ then
         9. Add $t(D)$ as last column to $M$;
         10. $O := O \cup \{t\}$;
         11. $S :=$ corner set of $O \cup \{t\}$;
         12. Append $O$ to list $HL$;
         13. $L, O, S, M, HL :=$ AllOIStep($L, O, S, M, HL$);
      14. end
   15. end
3. end
5. if Maxbool == TRUE then Append $O$ to list $L$;
6. end
7. return $L, O, S, M, HL$;
\[ O_1 = \{1, X_1, X_2, X_1X_2\} \text{ and } O_2 = \{1, X_1, X_2, X_2^2\}. \] This design lies very close to the 2\(^2\)-full factorial design \( \hat{D} = \{(1, 1), (1, -1), (-1, 1), (-1, -1)\} \) which famously has only \( O_1 \) in its statistical fan. Hence the numerical statistical fan of the noisy design \((D, \delta)\) should also only contain \( O_1 \) for any tolerance vector \( \delta \) with sufficiently big \(||\delta||\). Indeed, applying Algorithm 3 to \((D, \delta)\), we get \( S_{\text{num}}(D, \delta) = O_1 \) for all \( \delta = (0, \delta_{X_2}) \) with \( \delta_{X_2} \geq 1/2000 = 0.0005 \). Note that here the critical value of \(||\delta||\) is roughly the range of each component divided by \( c(\Omega_{O_2}(D)) = 4001 \).

The next example compares Algorithm 3 with the NMB algorithm (Fassino, 2010).

**Example 6.** (Example 6.4 in Fassino (2010)). Consider the empirical design \((D, \delta)\) with \( D = \{(1, 6), (2, 3), (2.449, 2.449), (3, 2), (6, 1)\} \) and \( \delta = 0.018 \cdot (1, 1) \). The NMB algorithm (with term order DegLex) computes only the stable order ideal \( O = \{1, X_1, X_2, X_2^2, X_3^2\} \). Our algorithm 3 computes the numerical statistical fan \( S_{\text{num}}(D, \delta) = \{\{X_1^2, X_2^2\}, \{X_1^3, X_2\}, \{X_1, X_2^3\}, \{X_1^2\}, \{X_2^3\}\} \) where we displayed for each order ideal only its maximal elements, e.g. \( \{X_1^2, X_2^2\} \) stands for the order ideal \( \{1, X_1, X_2, X_1^2, X_2, X_2^2\} \), and \( \{X_1, X_2^3\} \) represents the order ideal \( O \) computed by the NBM algorithm.

While the NMB algorithm computes only one stable order ideal (for a given term order), our Algorithm 3 computes them all. Even if we would run the NBM algorithm through all possible term orderings - which is a difficult task to implement - we could only compute the numerical algebraic fan \( A_{\text{num}}(D, \delta) \) (Rudak, Kuhnt and Riccomagno, 2016) which is a subset of \( S_{\text{num}}(D, \delta) \).

### 4 Application to thermal spraying data

We are going to compute the numerical statistical fan for real data coming from a High Velocity Oxygen Fuel (HVOF) thermal spraying process. Section 4.1 describes the data and the designs \( D_X \) and \( D_Y \) in question. In Section 4.2 we compute the numerical statistical fan \( S_{\text{num}}(D_Y, \delta) \) and compare it to the statistical fan \( S(D_Y) \).

All computations were performed using the computer algebra system MAGMA (Bosma, Cannon and Playoust, 1997).

#### 4.1 Data

In an HVOF process cermet powder particles are sprayed by a spraying gun to build a coating on a specimen. Controllable machine parameters (\( X \) variables) are varied accord-
ing to an experimental design $D_X$. In-flight properties ($Y$ variables) are measured during the process. Coating properties ($Z$ variables) are very time-consuming and expensive to measure as the specimen has to be destroyed. Thus it is desirable to predict coating properties on the basis of particle properties, i.e., we are considering models $Z = Z(Y)$. Table 1 displays all $X$, $Y$, and $Z$ variables involved.

While the other variables are self-explanatory, Lambda is defined as the quotient of actual oxygen-fuel mass ratio to its stoichiometric value. The experimental design $D_X$ is chosen as a $2^4$ factorial design with one center point, i.e., $D_X = \{ \pm 1 \}^4 \cup \{ 0 \in \mathbb{R}^4 \}$. The measured values of in-flight properties form a noisy design $D_Y \subset \mathbb{R}^4$ with $|D_Y| = |D_X| = 17$. Figure 2 displays the design $D_X$ and the corresponding values in the design $D_Y$. Since we can only draw a perspective plot of 3 dimensions, the 4-th dimension in these 4-dimensional designs $D_X, D_Y$ was either displayed by different symbols for different levels (for kerosene in $D_X$) or by using a continous color spectrum (for temperature in $D_Y$).

The numbers $i = 1, \ldots, 17$ label corresponding design points $p_i \in D_X$ and $q_i \in D_Y$, i.e. the data point $q_i \in D_Y$ is the result from a measurement with process parameters given by $p_i \in D_X$.

### 4.2 Computation of the statistical fans

Since the system which measures the particle and flame properties records data every second, we were able to estimate a bound for the standard deviation for every data point and in-flight property. We took the maximum over all data points (for each in-flight property) and chose $\delta_i = 2 \cdot \sigma_i^{(\text{max})}$ for $i \in \{T, V, W, I\}$. This procedure led to the tolerance vector $\delta = (\delta_T, \delta_V, \delta_W, \delta_I) = (12.5, 7, 0.3, 1.5)$. We check that all empirical points of the noisy design $(D_Y, \delta)$ are well separated for this choice of $\delta$ which is indeed the case. If this were not the case we could first apply a data reduction step where we merge points that are contained in each others $\delta$-boxes. Explicit algorithms for such data reduction are given in Torrente (2009).

| process parameters $X$ | in-flight properties $Y$ | coating properties $Z$ |
|------------------------|--------------------------|------------------------|
| Kerosene               | Temperature ($T$)         | Porosity               |
| Lambda                 | Velocity ($V$)           | Hardness               |
| Stand-off Distance     | Flame width ($W$)        | Thickness              |
| Feeder Disc Velocity   | Flame intensity ($I$)     | Deposition efficiency  |
Figure 2: Designs $D_X$ and $D_Y$ with corresponding design points enumerated.

We compute the numerical statistical fan $S_{num}(D_Y, \delta)$ of the noisy design $(D_Y, \delta)$ using Algorithms 3 and 4. We find that $S_{num}(D_Y, \delta)$ has 45 maximal order ideals of different cardinality, i.e. the hierarchical models vary in number of effects.

To explore the resulting models further, we look at the condition numbers of the design matrices as an alternative characteristic of stability. Since the condition number is not invariant under scaling and translation of the coordinates of the design points, we standardize our design $D_Y$ such that the range of each in-flight property is exactly $[-1, 1]$. This makes no difference when computing the numerical fan since the heuristical Fassino condition is invariant under scaling and translation of each coordinate according to Theorem 4.1 in Fassino (2010). The condition numbers of the design matrices turn out to be reasonably small. The largest condition number is $c(X_{O}(D)) = 62.25$ for $O = \{T^2V, V^5\}$ (only maximal elements displayed), and the smallest condition number is $c(X_{O'}(D)) = 5.65$ for $O = \{TW, V^2, W^2\}$. For models with high degree terms as $V^5$ we expect higher condition numbers. The reason why we cannot get close to 1 are design points which are well separated by $\delta$ but still quite close to each other (take a look at $D_Y$ in Figure 2).

The next step in a statistical data analysis would be to use these hierarchical models in a model selection procedure. Here, we focus on some properties of our approach instead. One question might be how the size of the numerical statistical fan changes when the $\delta$-vector becomes smaller. Table 2 displays the size of the numerical statistical fan $S_{num}(D_Y, k\delta)$ for $\delta = (12.5, 7, 0.3, 1.5)$ and different scale factors $k$. Additionally, we also give the number of all stable order ideals and all weakly maximal among them.
Table 2: Number of (maximal) stable order ideals of the empirical design \((D_Y, k\delta)\) for \(\delta = (\delta_T, \delta_V, \delta_W, \delta_I) = (12.5, 7, 0.3, 1.5)\) and different scales \(k\)

| scale \(k\) | \(|S_{num}(D_Y, k\delta)|\) | \(#\{\text{weakly max. OIs}\}\) | #stable order ideals |
|---|---|---|---|
| 2 | 5 | 10 | 30 |
| 1.5 | 11 | 22 | 97 |
| 1.2 | 25 | 44 | 210 |
| 1 | 45 | 68 | 481 |
| 0.9 | 77 | 103 | 777 |
| 0.8 | 165 | 230 | 1551 |
| 0.7 | 342 | 511 | 3079 |
| 0.6 | 697 | 974 | 6740 |
| 0.5 | 1488 | 2086 | 16233 |

Table 3: Maximal Stable order ideals by cardinality in numerical statistical fan \(S_{num}(D_Y, k\delta)\) for \(\delta = (\delta_T, \delta_V, \delta_W, \delta_I) = (12.5, 7, 0.3, 1.5)\) and different scales \(k\).

| \(k\) vs. \(|\mathcal{O}|\) | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | sum |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 2 | - | 1 | 2 | 2 | - | - | - | - | - | - | - | - | - | - | - | 5 |
| 1.5 | - | 1 | 3 | 3 | - | 3 | 1 | - | - | - | - | - | - | - | - | 11 |
| 1.2 | - | - | - | 3 | 8 | 10 | 3 | - | - | 1 | - | - | - | - | - | 25 |
| 1 | - | - | - | 2 | 6 | 9 | 7 | 8 | 9 | 4 | - | - | - | - | - | 45 |
| 0.9 | - | - | - | - | 1 | 6 | 21 | 18 | 11 | 20 | - | - | - | - | - | 77 |
| 0.8 | - | - | - | - | 13 | 19 | 37 | 37 | 35 | 24 | - | - | - | - | - | 165 |
| 0.7 | - | - | - | - | 2 | 17 | 50 | 103 | 80 | 71 | 16 | 3 | - | - | - | 342 |
| 0.6 | - | - | - | - | 5 | 2 | 21 | 119 | 184 | 215 | 120 | 31 | - | - | - | 697 |
| 0.5 | - | - | - | - | - | 3 | 34 | 168 | 381 | 487 | 315 | 95 | 5 | - | - | 1488 |

As expected \(|S_{num}(D_Y, \delta)|\) becomes larger for smaller scale factor \(k\), because numerical aliasing becomes less likely for smaller \(\delta\)-boxes.

To get an impression of which sizes of the numerical statistical fan occur, we display the number of occurrences of maximal stable order ideals with different cardinalities in Table 3.

We observe that for smaller scale, i.e. higher precision, the sizes of the stable order ideals increase. Indeed, in the limit \(k \to 0\), \(S_{num}(D_Y, \delta)\) becomes the usual statistical fan \(S(D_Y)\) and the sizes of the stable order ideals become \(|D_Y|\).
Table 4: Comparison of numerical and statistical fan sizes

| $|D_Y|$ | $S_{\text{num}}(D_Y, \delta)$ | #stable OIs | $|S(D_Y)|$ | #OIs | $p_d(n)$ | $p_d(\leq n)$ |
|-------|-----------------|------------|-----------|-------|----------|---------------|
| 17    | 45              | 481        | 416570    | 847078| 416849   | 847517        |
| 16    | 39              | 402        | 213954    | 430495| 214071   | 430668        |
| 15    | 45              | 425        | 108752    | 216529| 108802   | 216597        |
| 14    | 34              | 339        | 54791     | 107777| 54804    | 107795        |
| 13    | 33              | 317        | 27235     | 52973 | 27248    | 52991         |
| 12    | 34              | 298        | 13413     | 25725 | 13426    | 25743         |
| 11    | 24              | 206        | 6487      | 12299 | 6500     | 12317         |
| 10    | 22              | 191        | 3109      | 5799  | 3122     | 5817          |
| 9     | 33              | 179        | 1451      | 2677  | 1464     | 2695          |
| 8     | 21              | 118        | 680       | 1226  | 684      | 1231          |

We also compare the sizes of the numerical statistical fan $S_{\text{num}}(D_Y, \delta)$ to the statistical fan $S(D_Y)$. Table 4 shows the size of the numerical statistical fan (for $\delta = (12.5, 7, 0.3, 1.5)$) and for the statistical fan whose cardinality grows exponentially with the size of the design. Here, we successively deleted arbitrary points from the design with $|D_Y| = 17$. Furthermore, we also computed the number of all hierarchical models with $n$ (and with $\leq n$) terms, denoted by $p_d(n)$ and $p_d(\leq n)$, respectively. For $d = 4$ they correspond to so-called solid partitions. Recall that there is no generating function of $p_d(n)$ known for $d \geq 4$. First enumerations of the number of solid partitions were done in Atkin et al. (1967) and Knuth (1970).

We observe that the numerical statistical fan is significantly smaller than the statistical fan, i.e. it is effectively computable. Furthermore, its size does not grow (sub-)exponentially with the design size. The size of the statistical fan of $D_Y$ turns out to be only a bit smaller than number of all maximal hierarchical models $p_d(n)$. Similarly, the number of all order ideals identifiable by $D_Y$ is only a few less than the number of all hierarchical models (with less than $n$ terms). This shows that $D_Y$ is close to a truly generic design where we would expect that $|S(D_Y)|$ and $p_d(n)$ coincide.

5 Discussion and Outlook

The computation of the numerical fan $S_{\text{num}}(D, \delta)$ provides improved model selection through the enhanced knowledge of the space of all identifiable stable hierarchical mod-
els that avoid "numerical aliasing". In stark contrast to the statistical fan of a generic design, the numerical fan turns out to be effectively computable - at least for small data sets with few dimensions. The recursive enumeration of the numerical fan $S_{num}(D, \delta)$ can be combined with subset selection by considering only submodels that contain the new monomial $t$ to be included to an order ideal $\mathcal{O}$. Maximal Models can also be roughly ordered according to their validity by scaling the tolerance vector.

In future work we may consider an extension to other model classes like quasi-order ideals \cite{Mourrain2012}. The recursive algorithm can be used to search for low degree polynomials that describe varieties close to all empirical points. Indeed, every numerical linear dependence provides such polynomial equations. Recall that the Fassino condition (with $\delta^2$-term) is only a sufficient condition for numerical independence. If it is not fulfilled, we may search for a perturbed design providing linear dependence of design vectors. Such a search algorithm was suggested in \cite{Fassino2013}.

Acknowledgements

The financial support of the Deutsche Forschungsgemeinschaft (SFB 823, project B1) is gratefully acknowledged.

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