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Polynomial Ideals, Monomial Bases and a Divided Difference Formula

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Summary. - *A generalised (multivariate) divided difference formula is given for an arbitrary finite set of points with no subsets of three points that lie on a line. This follows from an extension of the Newton's polynomials and Newton's interpolation formula. It is derived as the interpolation based on Gröbner bases for the grid expressed as a zero-dimensional variety and is typically dependent on the chosen term-ordering and the selected ordering of points in the grid.*

1. Introduction

This paper derives from recent joint work by the authors and others on using Gröbner bases in experimental design and interpolation, see Pistone, Riccomagno and Wynn (2001) [5, 7] and Fontana, Pistone and Rogantin (2000) [15]. In particular experimental designs, that

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is sets of observation points, or grids for interpolation, are expressed as zero-dimensional varieties and interpolators as elements of the quotient space with respect to the corresponding polynomial ideal.

The polynomial interpolators, expressed as remainders, are in a well-defined sense unique and also give a neat generalisation of Newton's divided difference interpolation formula. This paper applies these initial ideas to general grids using computational commutative algebra and algebraic geometry.

For related results and approaches see de Boor and Ron (1992) [4] expecially from a numerical analysis standpoint, Buchberger and Möller (1982) [13] for a first approach based on Gröbner bases, Möller (1998) [12], Gasca and Sauer (2000) [8] for a recent survey and references therein.

2. Newton's interpolation formula

We start by recalling some results on divided differences in one dimension. See Hildebrand (1956) [9, Sec. 2.2]. Let $v_0, \ldots, v_n$ be $n+1$ distinct real numbers and define the Newton polynomials

$$\begin{cases} g_0(v) = 1 \\ g_1(v) = v - v_0 \\ \quad \vdots \\ g_n(v) = (v - v_0)(v - v_1) \ldots (v - v_{n-1}) \\ g_{n+1}(v) = (v - v_0)(v - v_1) \ldots (v - v_n) \end{cases} \tag{1}$$

Let $f(v)$ be a function on $\mathbb{R}$ and define the divided differences

$$\begin{aligned} f[v_0] &= f(v_0) \\ f[v_0, v_1] &= \frac{f[v_1] - f[v_0]}{v_1 - v_0} \end{aligned}$$

and by induction

$$f[v_0, \ldots, v_k] = \frac{f[v_1, \ldots, v_k] - f[v_0, \ldots, v_{k-1}]}{v_k - v_0}.$$

It can be checked by induction that

$$f[v_0, \ldots, v_k] = \sum_{j=0}^{k} \frac{f(v_j)}{\prod_{i=0, i \neq j}^{k} (v_j - v_i)}. \tag{2}$$

This formula shows that while usually $v_0 < v_1 < \ldots < v_n$ is assumed, (2) is invariant under permutations of points, that is the divided difference of f at $v_0, \ldots, v_k$ depends only on the set $D_{k+1} = \{v_0, \ldots, v_k\}$. In the multi-dimensional case below we will use the reverse notation $[v_0, \ldots, v_k]f$ to stress the interpretation of divided differences as operators acting on f.

The Newton's interpolation formula is obtained by the previous divided difference formula applied to $\{v_0, \ldots, v_k, v\}$ (see [9, Sec. 2.5])

$$f(v) = f[v_0] + g_1(v) f[v_0, v_1] + \ldots + g_n(v) f[v_0, \ldots, v_n] + R(v). \tag{3}$$

For the error we have

$$R(v) = g_{n+1}(v) f[v_0, \ldots, v_n, v] = g_{n+1}(v) \frac{f^{(n+1)}(\xi)}{(n+1)!} \tag{4}$$

with $\xi \in (v_0, v_n)$ ($v_0 < v_i < v_n$ for all $i = 1, \ldots, n-1$) and $R(v_i) = 0$ ($i = 0, \ldots, n$) (see [9, Sec. 2.6]).

In the next sections we generalise the above to an arbitrary finite set of points in $\mathbb{R}^d$ using Gröbner bases and algebraic geometry methods. As working examples we consider five types of grids, the fourth one being a generalisation of the first three. For n_j nonnegative integer ($j = 1, \ldots, d$) the *product grid* is

$$\prod_{j=1}^{d} \{0, \ldots, n_j - 1\}.$$

Product grids are classically considered in textbooks, see Isaacson and Keller (1966) [10]. For $n \in \mathbb{Z}_{>0}$ the *triangular grid* is

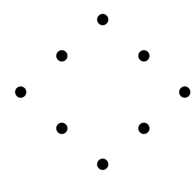
$$\left\{ v \in \mathbb{Z}^d : v_i \geq 0 \text{ and } 0 \leq \sum_{i=1}^{d} v_i \leq n \right\}.$$

The *echelon grid* is the complement of a finitely generated positive integer lattice. The *generalized echelon grid* is obtained as union of an echelon grid and all the rotations along the coordinate axes.

In design of experiment literature the grid below is sometimes called a *composite design*

$$\Big\{v \in \mathbb{Z}^d : \begin{array}{rcl} |v_i| & = & 1 \text{ for } i = 1, \ldots, d; \text{ or} \\ |v_j| & = & 2 \text{ and } v_i = 0 \text{ for all } i \neq j \text{ and } i = 1, \ldots, d \end{array} \Big\}$$

(see Box and Wilson, 1951 [2]). An example is



3. Using Gröbner bases

We refer to Cox, Little and O'Shea (1997) [3], Adams and Loustaunau (1994) [1] and Kreuzer and Robbiano (2000) [11] for the fundamentals of computational commutative algebra.

Gröbner bases provide a special way to write a finite system of polynomial equations. They depend on a term-ordering on the set of terms, equivalently a total ordering on the grid of integer vectors with non-negative components in $\mathbb{R}^d$ (with d positive integer), and they allow a nice interpretation of properties such as interpolation. An integer vector in $\mathbb{R}^d$ with non-negative components can be viewed as the exponent of a term, or power product, in d-indeterminates. Thus to fix notation, $\alpha \in \mathbb{Z}^d_{\geq 0}$ corresponds to the term $x^\alpha = x_1^{\alpha_1} \ldots x_d^{\alpha_d}$, in particular $\alpha = 0_d \in \mathbb{R}^d$ corresponds to 1.

Definition 3.1. *A term-ordering τ is a total ordering $x^\alpha \prec_\tau x^\beta$ of terms compatible with simplification of terms: $x^\alpha \prec_\tau x^\beta$ implies that $x^{\alpha+\gamma} \prec x^{\beta+\gamma}$ for $\alpha, \beta, \gamma \in \mathbb{Z}^d_{\geq 0}$.*

Note that $1 \prec_\tau x^\alpha$ for all α in $\mathbb{Z}^d_{\geq 0}$.

The two basic term-orderings are the lexicographic term-ordering and the degree reverse lexicographic term-ordering, denoted respectively by `plex` and `tdeg`. Both imply an initial order on the variables, say $x_1 \succ x_2 \succ \ldots \succ x_d$. The first one orders the exponents of the monomials lexicographically

$$x^\alpha \succ x^\beta \quad \text{if and only if} \quad \begin{cases} \alpha_1 > \beta_1 \text{ or} \\ \text{there exists } p \leq d \text{ such that } \alpha_i = \beta_i \\ \ \text{for } i = 1, \dots, p-1 \text{ and } \alpha_p > \beta_p \end{cases}$$

and the second one first orders by total degree (sum of the exponents)

$$x^\alpha \succ x^\beta \quad \text{if and only if} \quad \begin{cases} \sum_{i=1}^d \alpha_i > \sum_{i=1}^d \beta_i \text{ or} \\ \text{there exists } p \leq d \text{ such that} \alpha_i = \beta_i \\ \text{for } i = p+1, \dots, d \text{ and } \beta_p > \alpha_p. \end{cases}$$

A term-ordering can be reduced to a `plex` ordering using the fact that each ordering corresponds to a (non unique) array of integer vectors (see Robbiano, 1985 [16], and Adams and Loustaunau, 1994 [1]). The use of orderings to emphasize the relative importance of groups of variables is shown in Pistone, Riccomagno and Wynn [6].

Let $\mathbb{R}[x_1, \dots, x_d]$ be the set of all polynomials in $x_1, \dots, x_d$ and with real coefficients. A set of polynomials $I \subset \mathbb{R}[x_1, \dots, x_d]$ is a polynomial ideal if (i) $f + g \in I$ for all $f, g \in I$ and (ii) $sf \in I$ for all $f \in I$ and $s \in \mathbb{R}[x_1, \dots, x_d]$. The polynomial ideal generated by the polynomials $f_1, \dots, f_r \in \mathbb{R}[x_1, \dots, x_d]$ is

$$I = \left\{ f \in \mathbb{R}[x_1, \dots, x_d] : f = \sum_{i=1}^r s_i f_i \text{ where } s_i \in \mathbb{R}[x_1, \dots, x_d] \right\}$$

and is denoted by $I = \langle f_1, \dots, f_r \rangle$.

The leading term of a polynomial $f \in \mathbb{R}[x_1, \dots, x_d]$ with respect to the term-ordering τ, $\mathrm{Lt}_\tau(f)$ is the largest term in f with respect to τ.

DEFINITION 3.2. *Let I be a polynomial ideal in $\mathbb{R}[x_1, \dots, x_d]$ and let $G = \{g_1, \dots, g_s\}$ be a subset of I. The set G is a Gröbner basis for I with respect to the term-ordering τ if and only if*

$$\langle \mathrm{Lt}_\tau(g_1), \dots, \mathrm{Lt}_\tau(g_s) \rangle = \langle \mathrm{Lt}_\tau(f) : f \in I \rangle.$$

That is the ideal of the leading terms of I is generated by the finite set of leading terms of the elements in the Gröbner basis G. A Gröbner basis, G is *reduced* if for all $g \in G$ the coefficient of the leading term of g is one and no term of g lies in $\langle \mathrm{Lt}_\tau(f) : f \in G \setminus \{g\}\rangle$. Given a term-ordering the reduced Gröbner basis of a polynomial ideal is unique. See Cox, Little and O'Shea (1997) [3, Sec. 2.7].

Let D be a finite set of distinct points in $\mathbb{R}^d$, called a design or a grid. The ideal associated with D, called *design ideal* or *ideal of points* and indicated with $\mathrm{Ideal}\,(D)$, is the set of all polynomials whose zeros include the design points. There are algorithms and softwares that given in input D and a term-ordering τ return the reduced Gröbner basis of $\mathrm{Ideal}\,(D)$ with respect to τ.

A key notion is that of the quotient space of all polynomials by the design ideal. This quotient space is ring-isomorphic to the set of functions defined over D and called $\mathcal{L}(D)$. This is a vector space over the coefficient field, $\mathbb{R}$. A vector space basis is computed as all those terms not divisible by the leading terms of the Gröbner basis for the design ideal. It has the property that if a term x^α is in the vector space basis then all the terms that divide x^α are in the vector space basis. Vector space bases of the quotient space are indicated as $\mathrm{Est} = \{x^\alpha : \alpha \in L\}$ or $B(D)$. A first application of these ideas in statistics is to use the vector space basis to model the mean of a linear regression model identifiable by the design D (see Pistone and Wynn, 1996 [14]).

Different term-orderings lead to different Gröbner bases and thus to different vector-space bases of the quotient space. However, in certain cases the Gröbner basis is the same for all term-orderings. In this case we say that the Gröbner basis is *total*. This is the case for generalised echelon designs.

The design ideal is then the set of all polynomials interpolating the design points at zero. The closets in the quotient space modulo the design ideal represent the set of polynomials that have the same values at each point of the grid. That is, when we divide the polynomial f by the Gröbner basis G, we have

$$f(x) = \sum_{i=1}^{s} s_i(x) g_i(x) + r(x) \tag{5}$$

where $r(v) = f(v)$ for all $v \in D$ and r is the polynomial interpolating D. See Cox, Little and O'Shea (1997) [3].

We shall use the following theorem for whose proof we refer to Pistone, Riccomagno and Wynn (2001) [5].

THEOREM 3.3. *Let τ be a term-ordering and D a finite set of distinct points in $\mathbb{R}^d$. Let $G(D)$ be the unique reduced Gröbner basis of D with respect to τ, $\mathrm{Lt}(D)$ the set of leading terms of the polynomials in $G(D)$ and let $\mathrm{Est}(D) = \mathrm{Est}_\tau(D)$ be the unique monomial basis defined by $\mathrm{Lt}(D)$. Consider $\omega \in \mathbb{R}^d \setminus \{D\}$ and $D' = D \cup \{\omega\}$. Then,*

1. $\mathrm{Est}(D') = \mathrm{Est}(D) \cup \{x^\gamma\}$,
2. *$G(D)$ contains a polynomial $g_{D;\omega}$ whose leading term is x^γ,*
3. *$g_{D;\omega}(\omega) \neq 0$ and $g_{D;\omega}(v) = 0$ for all $v \in D$.*

Note that given the term-ordering and a point there is only one $g_{D,\omega}$.

4. A generalisation of Newton's polynomials

Let us now introduce an order on the points of D, so that D becomes the list of points $(v_0, \dots, v_n)$. The idea is to start with the empty-set and construct the design, D iteratively by adding a point at a time. In general, the construction and results we give depend on a term-ordering τ, which we assume given. Echelon grids are particularly pleasant as the construction and results do not depend on the chosen term-ordering. But they still depend on the order in which the design points are added.

We need some notations based on Theorem 3.3.

1. By recursively adding new points in the chosen order, we get the list of designs
$$D_k = \{v_0, \dots, v_{k-1}\}, \quad k \geq 1,$$
and $D_0 = \emptyset$.
2. To each design D_k a unique reduced Gröbner basis
$$G_k = G(\{v_0, \dots, v_{k-1}\}) = G(D_k), \quad k \geq 1,$$
is associated. The basis of the empty design is $G_0 = \{1\}$.

3. To each Gröbner basis G_k a unique list of monomials

$$B_{k+1} = \mathrm{Est}\left(\{v_0, \ldots, v_{k-1}\}\right) = B(D_k), \quad k \geq 1,$$

is associated. This list forms a linear basis of the vector space of responses $\mathcal{L}(D_k)$.

4. By adding a point at a time, from Theorem 3.3(1) we know a list of multi-exponents, $L = (\alpha_0, \alpha_1, \ldots, \alpha_k)$, $\alpha_0 = 0_d$, such that $B_k = \{x^{\alpha_0}, x^{\alpha_1}, \ldots, x^{\alpha_k}\}$.

   The position of α_i, $i = 0, \ldots, k$, in L might be different from the position given by the ordering of the x^{α_i} according to the term-ordering τ.

5. By Theorem 3.3(2), from each G_k we can single out a polynomial $g_k = g_{D_k;v_k}$ with $\mathrm{Lt}(g_k) = x^{\alpha_k}$. When we need to highlight the fact that the leading term of g_k is x^{α_k}, we use the notation g_{α_k}. Note that $g_0 = 1$ for all grids and term-orderings. We define

$$H_k = \{g_{D_i;v_i} : i = 0, \ldots, k\} = H(D_k).$$

With these notations in hand, we prove a result in linear algebra.

Theorem 4.1. *Let D be a finite set of $n+1$ distinct points in $\mathbb{R}^d$. Let an ordering of points in D and a monomial ordering τ be given. The set of polynomials $H(D) = \{g_k : k = 0, \ldots, n\}$ form a linear basis of $\mathcal{L}(D)$.*

Proof. The dimension as $\mathbb{R}$-vector space of $\mathcal{L}(D)$ is $n+1$ and the g_k's are $n+1$ and linearly independent as this sequence of identities prove. Let $\theta_k \in \mathbb{R}$ for all k. By the evaluation of $\sum_{k=0}^n \theta_k g_k(v) = 0$ in $v_i \in D$ we have $0 = \theta_i g_i(v_i)$, which implies $\theta_i = 0$ for all i as $g_i(v_i) \neq 0$ by construction and thus the linear independence of the g_i $(i = 0, \ldots, n)$ follows. □

Definition 4.2. *We will call the basis $H(D)$ in Theorem 4.1 a* generalised Newton, or g-Newton, basis*.*

To indicate the order on the points of D_k sometimes we write $g_{0,\ldots,k-1;k}$ instead of g_k. We illustrate the algorithm embedded in Theorem 4.1 in the case of our fundamental examples.

Triangular

For any term-ordering, for the grid $D_2 = ((0,0),(1,0),(0,1))$ the Gröbner basis is $G_2 = \{x_1^2 - x_1, x_2^2 - x_2, x_1x_2\}$ with $B_3 = \{1, x_1, x_2\}$. For $\omega = (1,1)$ we have $g_4 = x_1x_2$ and $\mathrm{Lt}(g_4) = x_1x_2$.

Product

For any term-ordering, for the grid $D_3 = ((0,0),(1,0),(0,1),(1,1))$ the Gröbner basis is $G_3 = \{x_1^2 - x_1, x_2^2 - x_2\}$ and $B_4 = \{x_1x_2, x_2, x_1, 1\}$. For $\omega = (2,1)$ we have $g_4 = x_1^2 - x_1$ and $\mathrm{Lt}(g_4) = x_1^2$.

Echelon

For any term-ordering, for the echelon grid represented by the following diagram ($d = 2$)

$$\begin{array}{llll} \bullet & & & \\ \bullet & \bullet & \bullet & \\ \bullet & \bullet & \bullet & \bullet \end{array}$$

we have

$$\begin{aligned} G_7 = \{ \; & x_1(x_1-1)(x_1-2)(x_1-3), \\ & x_2x_1(x_1-1)(x_1-2), \\ & x_1x_2(x_2-1), \\ & x_2(x_2-1)(x_2-2)\} \end{aligned} \tag{6}$$

and the list of exponents of the terms in B_8 has the same structure of the echelon grid. For $\omega = (1,2)$ we have $g_8 = x_1x_2(x_2 - 1)$.

Composite

With respect to $\texttt{tdeg}(x_1 \succ x_2)$ the Gröbner basis for the grid $D_7 = [(1,1),(-1,1),(-1,-1),(1,-1),(2,0),(0,2),(-2,0),(0,-2)]$ is

$$\begin{aligned} G_7 = \{ \; & x_2^4 - 3/2x_1^2 - 11/2x_2^2 + 6, \\ & x_1x_2^3 - x_1x_2, \\ & x_1^2x_2 + 1/3x_2^3 - 4/3x_2, \\ & x_1^3 + 3x_1x_2^2 - 4x_1\} \end{aligned}$$

giving $B_8 = \{1, x_2, x_2^2, x_2^3, x_1, x_1x_2, x_1x_2^2, x_1^2\}$. For $\omega = (2,1)$ we have $g_9 = x_1^2x_2 + 1/3x_2^3 - 4/3x_2$.

The transformation of vector space bases from the monomials x^α, $\alpha \in L$, to the polynomials g_k, $k = 0, \ldots, n$, is driven by a special lower triangular type of matrix G. Indeed for all $k = 0, \ldots, n$, as $g_k(v) = 0$ for all $v \in D_k$ and $g_k(v_k) \neq 0$ by construction, we have

$$g_k(v) = \sum_{j=0}^{k} g_{kj} x^{\alpha_j} = \sum_{j=0}^{n} g_{kj} x^{\alpha_j}$$

with $g_{kj} = 0$ for al $j > k$. In matrix notation we can write

$$[g_k(v_i)]_{i,k} = \left[\sum_{j=0}^{n} g_{jk} v_i^{\alpha_j} \right]_{i,k} = Z \, [g_{jk}]_{j,k} \tag{7}$$

where Z is the design matrix for D and $\{x^\alpha : \alpha \in L\}$,

$$Z = [v^\alpha]_{v \in D, \alpha \in L} \, .$$

The triangular structure of the matrix that gives the transformation of vector space bases from the x^α's to the g_α's ($\alpha \in L$)

$$G = [g_{jk}]_{j,k} = [g_{\alpha\beta}]_{\alpha \in L, \beta \in L}$$

supports our definition of the g_α, $\alpha \in L$ as a generalisation of the Newton polynomials to the multi-dimensional case. In a more concise matrix notation reminiscent of linear regression notation, we write (7) as

$$Z_g = ZG$$

where $Z_g = [g_\alpha(v)]_{v \in D, \alpha \in L} = [g_k(v_i)]_{i,k}$.

Echelon grid

Let the points in the echelon grid of the previous example be ordered left to right and top to bottom. Then we have

$$\begin{cases} g_0 = g_{\emptyset;(0,0)} &= 1 \\ g_1 = g_{\{(0,0)\};(1,0)} &= x_1 \\ g_2 = g_{\{(0,0),(1,0)\};(2,0)} &= x_1(x_1-1) \\ g_3 = g_{\{(0,0),(1,0),(2,0)\};(3,0)} &= x_1(x_1-1)(x_1-2) \\ g_4 = g_{\{(0,0),(1,0),(2,0),(3,0)\};(0,1)} &= x_2 \\ g_5 = g_{\{(0,0),(1,0),(2,0),(3,0),(0,1)\};(1,1)} &= x_1x_2 \\ g_6 = g_{\{(0,0),(1,0),(2,0),(3,0),(0,1),(1,1)\};(2,1)} &= x_2x_1(x_1-1) \\ g_7 = g_{\{(0,0),(1,0),(2,0),(3,0),(0,1),(1,1),(2,1)\};(0,2)} &= x_2(x_2-1) \end{cases}$$

and thus

$$\begin{bmatrix} 1&0&0&0&0&0&0&0\\ 1&1&0&0&0&0&0&0\\ 1&2&2&0&0&0&0&0\\ 1&3&6&6&0&0&0&0\\ 1&0&0&0&1&0&0&0\\ 1&1&0&0&1&1&0&0\\ 1&2&2&0&1&2&2&0\\ 1&0&0&0&2&0&0&2 \end{bmatrix} =$$

$$\begin{bmatrix} 1&0&0&0&0&0&0&0\\ 1&1&1&1&0&0&0&0\\ 1&2&4&8&0&0&0&0\\ 1&3&9&27&0&0&0&0\\ 1&0&0&0&1&0&0&1\\ 1&1&1&1&1&1&1&1\\ 1&2&4&8&1&2&4&1\\ 1&0&0&0&2&0&0&4 \end{bmatrix} \begin{bmatrix} 1&0&0&0&0&0&0&0\\ 0&1&-1&2&0&0&0&0\\ 0&0&1&-3&0&0&0&0\\ 0&0&0&1&0&0&0&0\\ 0&0&0&0&1&0&0&-1\\ 0&0&0&0&0&1&-1&0\\ 0&0&0&0&0&0&1&0\\ 0&0&0&0&0&0&0&1 \end{bmatrix}$$

5. Representation of a function in the g-Newton basis

The coefficients in the representation of $f \in \mathcal{L}(D)$ with respect to the linear basis $H(D) = \{g_k : k = 0, \dots, n\}$ are linear in $f(v)$, $v \in D$, and the coefficient at g_k depends only on the points v_j for $j \leq k$. For this reason, we adopt the standard divided difference notation

$$f(v) = \sum_{k=0}^{n} ([v_0, \ldots, v_k]f)\ g_k(v), \tag{8}$$

where $[v_0, \ldots, v_k]f$, $k = 0, \ldots, n$, can be seen as an operator on $\mathcal{L}(D)$ and is our generalisation of the divided difference operator. In particular

$$[v_0, \ldots, v_k]g_h = \begin{cases} 1 \text{ if } k = h \\ 0 \text{ if } k \neq h. \end{cases}$$

Consider next a monomial x^{α_h} in the vector space basis $B(D)$ of $\mathcal{L}(D)$. Then for $v \in \mathbb{R}^d$

$$\begin{aligned} v^{\alpha_h} &= \sum_{k=0}^{n} [v_0, \ldots, v_k] x^{\alpha_h} g_k(v) \\ &= \sum_{k=0}^{k} [v_0, \ldots, v_k] x^{\alpha_h} g_k(v) \end{aligned}$$

as, by construction of the g_k we have

$$[v_0, \ldots, v_k] x^{\alpha_h} = \begin{cases} 0 & \text{if } k > h \\ 1 & \text{if } k = h \text{ as we work with} \\ & \text{a reduced Gröbner basis.} \end{cases}$$

This can be translated into matrix representation. For the monomial basis $B(D_k)$ ordered according to L we can write

$$\begin{aligned} Z = [v_i^{\alpha_j}]_{i,j} &= \left[\sum_{k=0}^{n} [v_0, \ldots, v_k] x^{\alpha_j} g_k(v_i) \right] \\ &= [g_k(v_i)]_{i,k} \left[[v_0, \ldots, v_k] x^{\alpha_j} \right]_{k,j}. \end{aligned}$$

Define $\Delta = \left[[v_0, \ldots, v_k] x^{\alpha_j} \right]_{k,j}$ and from (7) we have $Z = Z_g \Delta = ZG\Delta$ and thus

$$\Delta = G^{-1}.$$

Note that as G is a lower triangular matrix, so is Δ.

6. Generalised divided differences

As we compare different permutations of the list $v_0, \dots, v_n$, we revert to a more general notation (see Theorem 3.3, Item 2)

$$f(v) = \sum_{k=0}^{n} [v_0, \dots, v_k] f g_{0,\dots,k-1;k}(v)$$

for $v \in D$. In particular by the triangular structure of G, $f(v_0) = [v_0]f$ and $f[v_1] = f(v_1) = [v_0]f + [v_0, v_1]f g_{0;1}(v_1)$ and thus

$$[v_0, v_1] f g_{0;1}(v_1) = [v_1]f - [v_0]f.$$

We add the next point and have

$$[v_2]f = f(v_2) = [v_0]f + [v_0, v_1]f g_{0;1}(v_2) + [v_0, v_1, v_2] f g_{0,1;2}(v_2).$$

Thus

$$[v_0, v_1, v_2] f g_{0,1;2}(v_2) = [v_0, v_2] f g_{0;2}(v_2) - [v_0, v_1] f g_{0;1}(v_2).$$

By induction the following recursive construction for divided differences holds. This carries on to the general case through the following theorem where we recall the notation $D_k = \{v_0, \dots, v_{k-1}\}$.

THEOREM 6.1. *Let $\{v_0, \dots, v_{k+1}\}$ be distinct points, $D_k = \{v_0, \dots, v_{k-1}\}$ and τ a term-ordering. The divided difference $[v_0, \dots, v_{k+1}]f$ is computed as a difference as follows*

$$\begin{aligned} [D_{k-1}, v_k, v_{k+1}] f g_{D_k; v_{k+1}}(v_{k+1}) = & [D_{k-1}, v_{k+1}] f g_{D_{k-1}; v_{k+1}}(v_{k+1}) \\ & - [D_{k-1}, v_k] f g_{D_{k-1}; v_k}(v_{k+1}). \end{aligned} \tag{9}$$

Proof. Consider all the given points

$$\begin{aligned} f(v_{k+1}) = & \sum_{i=0}^{k} [v_0, \dots, v_i] f g_{0,\dots,i-1;i}(v_{k+1}) + \\ & + [v_0, \dots, v_{k+1}] f g_{0,\dots,k;k+1}(v_{k+1}) \end{aligned}$$

and next the sequence without v_k

$$\begin{aligned} f(v_{k+1}) = & \sum_{i=0}^{k-1} [v_0, \dots, v_i] f g_{0,\dots,i-1;i}(v_{k+1}) + \\ & + [v_0, \dots, v_{k-1}, v_{k+1}] f g_{0,\dots,k-1;k+1}(v_{k+1}). \end{aligned}$$

Equate the right-hand sides of the above two identities and after cancellation of terms up to $k-1$ in the summation, obtain

$$\begin{aligned}[v_0,\ldots,v_{k+1}]fg_{0,\ldots,k;k+1}(v_{k+1}) = -[v_0,\ldots,v_k]fg_{0,\ldots,k-1;k}(v_{k+1})+\\ +[v_0,\ldots,v_{k-1},v_{k+1}]fg_{0,\ldots,k-1;k+1}(v_{k+1}).\end{aligned}$$

□

Echelon design

For the echelon design with Gröbner basis given in Equation (6), the `tdeg`$(x_1 \succ x_2)$ term-ordering and a two dimensional function f we have

$$\begin{aligned}f(x_1,x_2) =& f(0,0) + \frac{f(1,0)-f(0,0)}{1}x_1+\\ &+\frac{f(2,0)-f(1,0)+f(0,0)}{2}x_1(x_1-1)\\ &+\frac{18f(3,0)-12f(2,0)-6f(1,0)}{6}x_1(x_1-1)(x_1-2)+\\ &+\frac{f(0,1)-f(1,0)}{1}x_2\\ &+\frac{f(1,1)-f(0,1)-f(1,0)+f(0,0)}{1}x_1x_2\\ &+\frac{4f(2,1)-2f(1,1)-2f(1,0)}{2}x_1x_2(x_1-1)\\ &+\frac{2^6f(0,2)-2^3f(0,1)+2^37f(0,0)}{2}x_2(x_2-1).\end{aligned}$$

Note that we needed to compute the extra polynomials $g_{D_{k-1};v_{k+1}}$.

Due to the dependence of the g_k on the order on the grid points a generalization of Equation (2) does not exist. See also Example 7.4.

7. Grid shrinking

Consider a grid $v_0,\ldots,v_n \in \mathbb{R}^d$, the corresponding design $D = \{v_0,\ldots,v_n\}$ and a further point x. Also, consider a function f analytic at the grid points with Taylor series

$$f(v) = \sum_\alpha \frac{1}{\alpha!}D^\alpha f(0)v^\alpha \tag{10}$$

where α ranges over the d-dimensional integer vectors with non-negative components and D^α indicates the α-derivative. From (8) applied to the points $v = v_0, \ldots, v_n, x$ we obtain

$$f(v) = \sum_{j=0}^{n} [v_0, \ldots, v_j] f \, g_{0,\ldots,j-1;j}(v) + [v_0, \ldots, v_n, x] f \, g_{0,\ldots,n;x}(v). \tag{11}$$

For $v = x$ the last term is a remainder term for the interpolation of the grid $v_0, \ldots, v_n$, that we can write as

$$R(x) = [v_0, \ldots, v_n, x] f g_{0,\ldots,n;x}(x).$$

From (9) in Theorem 6.1 we have

$$R_n(x) = [D_{n-1}, x] f \, g_{D_{n-1};x}(x) - [D_n] f \, g_n(x).$$

If no three points of D_{n-1}, v_n, x lie on a line, the g-Newton polynomials in the divided difference formula above are equal, that is $g_{D_{n-1};x}(x) = g_n(x)$. This is always the case in one dimension. In general dimension, it is sufficient that no polynomial in the Gröbner basis $G(D_{n-1})$ vanishes at v_n or x.

Now for some $\epsilon > 0$ consider δ, $0 < \delta < \epsilon$ and the shrunken grid $\delta v_0, \ldots, \delta v_n$. We assume that x is such that for all δ the g-Newton polynomial $g_{\delta v_0,\ldots,\delta v_n;x}$ does not depend on δ. Roughly, this means that the point x is in generic position with respect to the shrunken grid. A sufficient condition for the existence of a suitable ϵ is that no polynomial in the Gröbner basis $G(D)$ vanishes at x. Under this assumptions, it is easy to check the following equalities among polynomials

$$\begin{cases} g_{\emptyset;\delta v_0}(v) = 1 \\ g_{\delta v_0;\delta v_1}(v) = \delta^{|\alpha_1|} g_{v_0;v_1}\left(\dfrac{v}{\delta}\right) \\ \vdots \\ g_{\delta v_0,\ldots,\delta v_n;x}(v) = \delta^{|\alpha_{n+1}|} g_{v_0,\ldots,v_n;x}\left(\dfrac{v}{\delta}\right) \end{cases} \tag{12}$$

where, for the multi-exponent $\beta = (\beta_1, \ldots, \beta_d)$, we write the total degree as $|\beta| = \sum_{i=1}^{d} \beta_i$.

Thus, we can apply the interpolation formula (11) to the shrunken grid and using (11) for $w = \delta v_0, \ldots, \delta v_n, x$, we obtain

$$f(w) = \sum_{j=0}^{n} \delta^{|\alpha_j|}[\delta v_0, \ldots, \delta v_j] f \, g_{v_0,\ldots,v_{j-1};v_j}\left(\frac{w}{\delta}\right) + \delta^{|\alpha_{n+1}|}[\delta v_0, \ldots, \delta v_n, x] f \, g_{v_0,\ldots,v_n;x}\left(\frac{w}{\delta}\right). \quad (13)$$

In (13), as $\delta \to 0$, we must consider the limit of the divided differences and the limit of the g-Newton basis. In one dimension, as $\delta \to 0$ the limit of $\delta^{|\alpha_j|}[\delta v_0, \ldots, \delta v_j] f$ is the α_j-th derivative of f at 0 divided by $j!$, and the limit of the polynomial $g_{\delta v_0,\ldots,\delta v_{j-1};\delta v_j}(v)$ is v^{α_j}. The situation in dimension $d > 1$ is more complicated.

Let us recall that we have a list of exponents $L = (\alpha_0, \ldots, \alpha_n)$, a monomial basis $B(D) = \{v^{\alpha_j} : j = 0, \ldots, n\}$, and that given a term-ordering, as all polynomials, also the g-Newton polynomials can be written as a monic leading term plus a tail,

$$g_{v_0,\ldots,v_{k-1};v_k}(v) = v^{\alpha_k} + \sum_{j=0}^{k-1} g_{kj} v^{\alpha_j}, \qquad k = 0, 1, \ldots, n. \quad (14)$$

THEOREM 7.1. *Assume that there exists $\epsilon > 0$ such that for all $0 < \delta < \epsilon$ the g-Newton polynomials of the shrunken grid are given by (12). Moreover, assume that the term-ordering τ and the order of the grid points are such that the total degrees of the elements in the list L are non decreasing. Then:*

1. *At a generic point $v \in \mathbb{R}^d$,*

$$\lim_{\delta \to 0} g_{\delta v_0,\ldots,\delta v_{k-1};v_k}(v) = v^{\alpha_k} + \sum_{0 \le j \le k-1 : |\alpha_k| = |\alpha_j|} g_{kj} v^{\alpha_j}.$$

2. $$\lim_{\delta \to 0} [\delta v_0, \ldots, \delta v_k] f = \sum_{|\alpha| = |\alpha_k|} \frac{1}{\alpha!} D^\alpha f(0)[v_0, \ldots, v_k] x^\alpha.$$

   In the summation the terms with $\alpha = \alpha_j$ and $j < k$ are zero.

3.

$$\lim_{\delta\to 0}\left([\delta v_0,\ldots,\delta v_n,x]f\, g_{\delta v_0,\ldots,\delta v_n;x}(v)\right) =$$
$$\left(v^{\alpha_{n_1}} + \sum_{0\le j\le n:|\alpha_j|=|\alpha_{n+1}|} g_{n+1,j}v^{\alpha_j}\right)\lim_{\delta\to 0}\left[v_0,\ldots,v_n,\frac{x}{\delta}\right]f.$$

Proof. (1). From (12) and (13) we have

$$\begin{aligned} g_{\delta v_0,\ldots,\delta v_{k-1};v_k}(v) &= \delta^{|\alpha_k|}g_{v_0,\ldots,v_{k-1};v_k}\left(\frac{v}{\delta}\right)\\ &= \delta^{|\alpha_k|}\left(\left(\frac{v}{\delta}\right)^{\alpha_k} + \sum_{j=0}^{k-1} g_{kj}\left(\frac{v}{\delta}\right)^{\alpha_j}\right)\\ &= v^{\alpha_k} + \sum_{j=0}^{k-1}\delta^{|\alpha_k|-|\alpha_j|}g_{kj}v^{\alpha_j}\end{aligned}$$

and the limit follows.
(2). We consider the function f_δ defined as $f_\delta(v) = f(\delta v)$ and its g-Newton interpolation formula. For $v = v_0,\ldots,v_n$ we have from (11)

$$f_\delta(v) = f(\delta v) = \sum_{j=0}^{n}[v_0,\ldots,v_j]f_\delta\, g_{0,\ldots,j-1;j}(v).$$

If we substitute w/δ we obtain, for $w = \delta v_0,\ldots,\delta v_n$,

$$f(w) = \sum_{j=0}^{n}[v_0,\ldots,v_j]f_\delta\, g_{0,\ldots,j-1;j}\left(\frac{w}{\delta}\right). \qquad (15)$$

Comparing (13) and (15) we equate coefficients obtaining

$$[v_0,\ldots,v_j]f_\delta = \delta^{|\alpha_j|}[\delta v_0,\ldots,\delta v_j]f$$

for $j = 0,\ldots,n$

Consider the Taylor series of $f_\delta(v)$

$$f_\delta(v) = f(\delta v) = \sum_\alpha \frac{1}{\alpha!}D^\alpha f(0)\delta^{|\alpha|}v^\alpha.$$

From the linearity of the operator $[v_0, \ldots, v_k]$ we get, using the assumption that the sequence $|\alpha_j|$ is non decreasing,

$$
\begin{aligned}
[\delta v_0, \ldots, \delta v_k] f &= \delta^{|\alpha_k|}[v_0, \ldots, v_k] f_\delta \\
&= \sum_\alpha \delta^{|\alpha|-|\alpha_k|} \frac{1}{\alpha!} D^\alpha f(0)[v_0, \ldots, v_k] x^\alpha \\
&= \sum_{|\alpha|=|\alpha_k|} \frac{1}{\alpha!} D^\alpha f(0)[v_0, \ldots, v_k] x^\alpha \\
&\quad + \delta \sum_{|\alpha|>|\alpha_k|} \delta^{|\alpha|-|\alpha_k|-1} \frac{1}{\alpha!} D^\alpha f(0)[v_0, \ldots, v_k] x^\alpha.
\end{aligned}
$$

(3). It follows from (11) evaluated at the grid $v_0, \ldots, v_n, x/\delta$ and (13) evaluated at the grid $\delta v_0, \ldots, \delta v_n, x$. $\square$

EXAMPLE 7.2. *Consider $d = 2$, $v_0 = (0,0)$, $v_1 = (1,1)$, $v_2 = (1,0)$, $v_3 = (0,1)$, and any monomial ordering such that $x_1 \prec x_2$. Then we have*

$$
\begin{cases}
g_0(x_1, x_2) = 1 \\
g_1(x_1, x_2) = x_1 \\
g_2(x_1, x_2) = x_2 - x_1 \\
g_3(x_1, x_2) = x_1 x_2 - x_2
\end{cases}
$$

and

$$
\begin{cases}
\lim_{\delta \to 0} \delta^0 g_0\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = 1 \\
\lim_{\delta \to 0} \delta^1 g_1\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = x_1 \\
\lim_{\delta \to 0} \delta^1 g_2\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = x_2 - x_1 \\
\lim_{\delta \to 0} \delta^2 g_3\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = x_1 x_2.
\end{cases}
$$

On the other hand, with the point ordering $v_0 = (0,0)$, $v_1 = (1,0)$,

$v_2 = (0,1)$, $v_3 = (1,1)$, we have

$$\begin{cases} \lim\limits_{\delta\to 0} \delta^0 g_0\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = 1 \\ \lim\limits_{\delta\to 0} \delta^1 g_1\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = x_1 \\ \lim\limits_{\delta\to 0} \delta^1 g_2\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = x_2 \\ \lim\limits_{\delta\to 0} \delta^2 g_3\left(\frac{x_1}{\delta}, \frac{x_2}{\delta}\right) = x_1 x_2. \end{cases}$$

EXAMPLE 7.3. *Let us study now the effect of shrinking by δ on a two point grid, $(v_0, v_1) = ((v_{01}, v_{02}), (v_{11}, v_{12}))$. By definition and (6.1) we have*

$$\begin{aligned} [\delta v_0]f &= f(\delta v_0) \\ [\delta v_0, \delta v_1] f g_{\delta v_0;\delta v_1}(\delta v_1) &= [\delta v_1]f - [\delta v_0]f \\ &= f(\delta v_1) - f(\delta v_0). \end{aligned}$$

Now, $g_{v_0;v_1}$ is a linear form $x_i - v_{0i}$ where x_i is the smallest determinate in the term-ordering such that $v_{0i} \neq v_{01}$. Thus from (12) we can write

$$\begin{aligned} [\delta v_0, \delta v_1] f \delta(v_{1i} - v_{0i}) &= f(\delta v_1) - f(0) - (f(\delta v_0) - f(0)) \\ [\delta v_0, \delta v_1] f &= \left(\frac{f(\delta v_1) - f(0)}{\delta} - \frac{f(\delta v_0) - f(0)}{\delta}\right) \frac{1}{v_{1i} - v_{0i}}. \end{aligned}$$

As $\delta \to +\infty$ this converges to

$$\left(\frac{\partial f}{\partial v_1} - \frac{\partial f}{\partial v_0}\right) \frac{1}{v_{1i} - v_{0i}}$$

where $\frac{\partial f}{\partial v_j}$ is the directional derivative of f at zero with respect to v_j, $j = 0, 1$.

EXAMPLE 7.4. *We want to compute*

$$\begin{aligned} &\lim_{\delta\to 0} [\delta v_0, \delta v_1, \delta v_2, \delta v_3] f = D^{(1,1)} f(v_0) + \\ &\quad + \frac{1}{2} D^{(2,0)} f(v_0) [v_0, v_1, v_2, v_3] x_1^2 + \frac{1}{2} D^{(0,2)} f(v_0) [v_0, v_1, v_2, v_3] x_2^2 \end{aligned}$$

for the first design in Example 7.2 with the term-ordering $\mathtt{tdeg}(x_2 \succ x_1)$*. The second term in this sum is zero and from repeated application of Theorem 6.1 we have*

$$\begin{aligned}
-[v_0, v_1, v_2, v_3]x_1^2 &= [v_0, v_1, v_2, v_3]x_1^2 g_{012;3}(v_3) \\
&= [v_0, v_1, v_3]x_1^2 g_{01;3}(v_3) - [v_0, v_1, v_2]x_1^2 g_{01;2}(v_3) \\
&= \left([v_0, v_3]x_1^2 g_{0;3}(v_3) - [v_0, v_1]x_1^2 g_{0;1}(v_3)\right) g_{01;3}(v_3) \\
&- \left([v_0, v_2]x_1^2 g_{0;2}(v_2) - [v_0, v_1]x_1^2 g_{0;1}(v_2)\right) \frac{1}{g_{01;2}(v_2)} \\
&= \left(x_1^2(v_3) - x_1^2(v_0)\right) g_{01;3}(v_3) + \left(x_1^2(v_2) - x_1^2(v_0)\right) \\
&- \frac{x_1^2(v_1) - x_1^2(v_0)}{g_{0;1}(v_1)} = 0.
\end{aligned}$$

Similarly we have $[v_0, v_1, v_2, v_3]x_2^2 = 0$ *and thus*

$$\lim_{\delta \to 0}[\delta v_0, \delta v_1, \delta v_2, \delta v_3]f = \frac{\partial^2 f(v_0)}{\partial x_1 \partial x_2}.$$

Consider now the following order on the grid points $((0,0),(1,0),(0,1),(1,1))$*. For a function* f *we have*

$$\begin{aligned}
[v_0, v_1, v_2, v_3]f =& \left(f(v_3) - f(v_0)\right) g_{0;3}(v_3) g_{01;3}(v_3) \\
&- \frac{f(v_1) - f(v_0)}{g_{0;1}(v_1)} g_{01;3}(v_3) \\
&- \left(f(v_2) - f(v_0)\right) g_{0;2}(v_2) g_{01;2}(v_2) \\
=& f(v_3) - f(v_2) - f(v_1) + f(v_0)
\end{aligned}$$

and thus

$$\begin{aligned}
[v_0, v_1, v_2, v_3]x_1^2 &= 0 \\
[v_0, v_1, v_2, v_3]x_2^2 &= 0.
\end{aligned}$$

This gives

$$\lim_{\delta \to 0}[\delta v_0, \delta v_1, \delta v_2, \delta v_3]f = \frac{\partial^2 f(v_0)}{\partial x_1 \partial x_2}$$

as before. Instead with the order $((0,0),(1,1),(0,1),(1,0))$ *we have*

$$[v_0, v_1, v_2, v_3]f = f(v_3) - f(v_2) - f(v_1) + f(v_0)$$

and thus

$$[v_0, v_1, v_2, v_3]x_1^2 = 0$$
$$[v_0, v_1, v_2, v_3]x_2^2 = -2$$

giving

$$\lim_{\delta \to 0} [\delta v_0, \delta v_1, \delta v_2, \delta v_3]f = \frac{\partial^2 f(v_0)}{\partial x_1 \partial x_2} - \frac{1}{2}\frac{\partial^2 f(v_0)}{\partial x_2^2}.$$

This shows that the order in which the grid points are considered is relevant.

Theorem 7.1 gives minimal conditions under which the divided differences approximate appropriate linear combinations of mixed partial derivatives whose order is equal to the total degree of the leading term of the associated g-Newton polynomial. Special grids could give approximations of the single partial derivatives corresponding to the leading term, as Example 7.4 shows.

THEOREM 7.5. *Let the assumptions and notations be as in Theorem 7.1. Assume moreover that the g-Newton polynomials in (14) and the analogous polynomial $g_{D;x}(v)$ are such that the total degree of the leading term $|\alpha_k|$, $k = 0, \dots, n+1$, is strictly larger than the total degree of the other terms with non-zero coefficient. In other words, $j < k$ and $|\alpha_j| = |\alpha_k|$ implies $g_{kj} = 0$. Then:*

1. *At a generic point $v \in \mathbb{R}^d$,*

$$\lim_{\delta \to 0} g_{\delta v_0, \dots, \delta v_{k-1}; v_k}(v) = v^{\alpha_k}.$$

2.

$$\lim_{\delta \to 0} [\delta v_0, \dots, \delta v_k] f = \frac{1}{\alpha_k !} D^{\alpha_k} f(0).$$

3.

$$\lim_{\delta \to 0} \left([\delta v_0, \dots, \delta v_n, x] f g_{\delta v_0, \dots, \delta v_n; x}(v) \right) = \\ = v^{\alpha_{n+1}} \lim_{\delta \to 0} \left[v_0, \dots, v_n, \frac{x}{\delta} \right] f.$$

Proof. This follows from Theorem 7.1. ∎

8. Discussion

It has been the purpose of this paper to develop divided difference formulae for arbitrary grids and by contracting (shrinking) such grids obtain derivatives. At the heart of the construction is, as for more standard cases, interpolation. Gröbner basis theory, in which grids are considered zero-dimensional varieties, provides the machinery for the interpolation. But, the formulation depends on the term-ordering for the Gröbner basis and the special order in which the grid points are selected. Roughly, the latter order provides the sequence for the underlying recurrence relationship while the term-ordering, via the Gröbner basis, yields the actual polynomials from which the divided differences are constructed. For standard grids the two orders can be closely related whereas the present construction is quite general. Special constructions are a subclass.

If no three points in $\{0, \ldots, v_n, x\}$ lie on a line and α is sufficiently large, then $D^\alpha x^{\alpha_j} = 0$, $j = 0, \ldots, n$, implies

$$D^\alpha f(x) = D^\alpha \left([v_0, \ldots, v_n, x] f \, g_{n+1}(x) \right)$$

relating the remainder to the derivatives of f. This can be used to construct error formulae for Taylor approximation, of different kinds, but the full development of such formulae is the basis of ongoing research. Multivariate interpolation, together with the discussion of the evaluation of the remainder with the appropriate partial derivative is classically considered in case of regular grids, see for example [10, pp. 294–298].

In two dimensions, let us consider the product of two grids $x_0, x_1, \ldots, x_m$ and $y_0, y_1, \ldots, y_n$. For $i = 0, \ldots, m$, let $g_i(x) = \prod_{k=0}^{i-1} (x - x_k)/(x_i - x_k)$ be the normalised Newton polynomials for the x-grid. Similarly define $h_j(y) = \prod_{k=0}^{j-1} (y - y_k)(y_j - y_k)$. Then

$$g_i(x_u) h_j(y_v) = \begin{cases} 0 & \text{if } u < i \text{ and } v < j \\ 1 & \text{if } u = i \text{ and } v = j \end{cases}$$

is the tensor product of Newton polynomials $g_i h_j$ and it is a g-Newton sequence in our sense for the lexicographic term ordering. The same applies to any sub-grid of the product grid. The most commonly considered case is the triangular case.

As we have remarked in our discussion, in most cases the divided difference are approximations of linear combinations of partial derivatives, which in turn has an effect to the representation of the remainder. The easiest case is the triangular one: if partial derivatives up to order n are involved, then the remainder can be based on *all* partial derivatives of order $n+1$. In the rectangular case in [10] a remainder based on all "border" partial derivatives is given. This last result is, in our opinion, not optimal, as we expect a good representation of the remainder be based on the "minimal" elements of the complement of L. This is discussed in the literature of a different but related field, e.g. singularity theory. Our paper can be considered as a starting point in providing a coherent construction for derivatives.

Another avenue of research is the automation of the computations. Use should be made of fast algorithms for computing "ideals of points" for example available in CoCoA (version 4.1 freely available at http://cocoa.dima.unige.it at time of writing). Such developments are likely to fuse these symbolic computation methods with more standard numerical analysis and linear algebra techniques. A long term aim would be to aid numerical approximation and numerical differentiation over arbitrary grids. One motivation for the subject of experimental design is to minimize the number of observations to save cost. Interpreting "observations" as function evaluations it should be possible to use methods such as those of this paper to help cross-fertilize between numerical analysis and experimental design, which is typically considered as a branch of statistics.

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