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Hermite polynomial aliasing in Gaussian quadrature

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Grand plan

Determine classes of f polynomials, $\mathcal{D} = \{x_1, \ldots, x_n\}$ and $w = \{w_1, \ldots, w_n\}$ such that

$$\mathrm{E}(f(Z)) = \int_{\mathbb{R}} f(x) \frac{e^{-x^2/2}}{\sqrt{2\pi}} dx = \sum_{i=1}^{n} f(x_i) w_i$$

with $Z \sim \mathcal{N}(0, 1)$ using polynomial algebra and orthogonal polynomials.

Theorem

In one dimension, if

- $\mathcal{D}$ *are the zeros of the Hermite polynomial of degree* n
- w_i *is the expected values of the Lagrange polynomials*

$$l_i(x) = \prod_{i \neq j} \frac{x - x_i}{x_j - x_i}$$

- f *is a polynomial of degree smaller or equal to* $2n - 1$

then the equality holds.

Abstract and a reference

In the computational algebra approach to DoE, the set of design points is described as the solution of a system of polynomial equations and the identification of various classes of models is computed by the use of special bases of the corresponding polynomial ideal.

A recent overview of this new field, termed Algebraic Statistics, and the first mention of the application to polynomial chaos are in

- P. Gibilisco, E. Riccomagno, M. Rogantin, H.P. Wynn, eds., *Algebraic and Geometric Methods in Statistics*, Cambridge University Press, 2010.

Here we present the first results of a research in progress in which we explore the applicability of these ideas when the defining equations are derived from Hermite polynomials and when the calculus is Hermite polynomial based, to obtain a folding over a finite set of points of multivariate polynomials.

This is related to quadrature formulas and has strong links with designs of experiments. Hermite polynomials are key tools in many areas: chaos expansions, Malliavin calculus, SODE and SPDE, p-rough paths, ...

I. Hermite polynomials and Stein-Markov operator

Definition

1. Define $\delta f(x) = xf(x) - f'(x) = -e^{x^2/2}\frac{d}{dx}\left(f(x)e^{-x^2/2}\right)$. If $Z \sim \mathcal{N}(0,1)$

$$\mathrm{E}\left(g(Z)\delta^n f(Z)\right) = \mathrm{E}\left(d^n g(Z) f(Z)\right),$$

i.e. δ is the transpose of the derivative w.r.t. the standard Gaussian measure.

2. Define $H_0 = 1$, $H_n(x) = \delta^n 1$, $n > 0$, e.g.

$$H_1(x) = x, H_2(x) = x^2 - 1, H_3(x) = x^3 - 3x, H_4(x) = x^4 - 6x^2 + 3, \dots$$

Properties

1. The transposition formula shows that the H_n's are orthogonal
2. $d\delta - \delta d = \mathrm{id}$, $dH_n = nH_{n-1}$, $\mathrm{E}(H_n^2(Z)) = n!$, $H_{n+1} = xH_n - nH_{n-1}$.

- P. Malliavin, *Integration and probability*, Springer-Verlag, New York, 1995, with the collaboration of Hélène Airault, Leslie Kay and Gérard Letac, Edited and translated from the French by Kay, foreword by Mark Pinsky.

Theorem (Zeros of H_n)

1. *The Hermite polynomial H_n, $n \geq 1$, has n distinct real roots*
2. *which are separated by those of H_{n+1}.*

Theorem (Linear structure)

1. $\deg_x(H_n(x)) = n$.
2. $\mathrm{Span}(1, x, \ldots, x^n) = \mathrm{Span}(H_0, H_1(x), \ldots, H_n(x))$.

Theorem (Ring structure)

1. $H_k H_n = H_{n+k} + \sum_{i=1}^{n \wedge k} \binom{n}{i}\binom{k}{i} i! H_{n+k-2i}$, $n, k \geq 1$.
2. *If* $H_n(x) = 0$, *then* $H_{n+k}(x) + \sum_{i=1}^{n \wedge k} \binom{n}{i}\binom{k}{i} i! H_{n+k-2i}(x) = 0$, $n \geq 1$.

In statistical language, item 3 shows an aliasing relation on the design

$$\mathcal{D}_n = \{x \colon H_n(x) = 0\}$$

- W. Gautschi, *Orthogonal polynomials: computation and approximation*, Numerical Mathematics and Scientific Computation, Oxford University Press, New York, 2004.

Aliasing computation

- The computation of the normal form introduces a notion of confounding. For example from $H_{n+1}(x) = xH_n(x) - nH_{n-1}(x)$ we obtain $H_{n+1}(x) \equiv -nH_{n-1}(x)$ where $\equiv$ stands for equality over $\mathcal{D}_n = \{x : H_n(x) = 0\}$, that is remainder of division by H_n.
- In general let $H_{n+k} \equiv \sum_{j=0}^{n-1} h_j^{n+k} H_j$ be the representation of H_{n+k} at $\mathcal{D}_n$. Substitution in the product formula gives

$$\begin{aligned} \mathrm{NF}(H_{n+k}) &\equiv -\sum_{i=1}^{n \wedge k} \binom{n}{i} \binom{k}{i} i! \, \mathrm{NF}(H_{n+k-2i}) \\ &= -\sum_{i=1}^{n \wedge k} \binom{n}{i} \binom{k}{i} i! \sum_{j=0}^{n-1} h_j^{n+k-2i} H_j \end{aligned}$$

Equating coefficients gives a general recursive formula

$$h_j^{n+k} = -\sum_{i=1}^{n \wedge k} \binom{n}{i} \binom{k}{i} i! \, h_j^{n+k-2i}$$

The first confounding relationships are

k	expansion
1	$-nH_{n-1}$
2	$-n(n-1)H_{n-2}$
3	$-n(n-1)(n-2)H_{n-3} + 3nH_{n-1}$
4	$-n(n-1)(n-2)(n-3)H_{n-4} + 8n(n-1)H_{n-2}$
5	$-\frac{n!}{(n-5)!}H_{n-5} + 5nH_{n-1} + 15n(n-1)(n-2)H_{n-3}$
6	$-\frac{n!}{(n-6)!}H_{n-6} + 24n(n-1)(n-2)(n-3)H_{n-4} + 10n(n-1)(2n-5)H_{n-2}$

- For $f = \sum_{i=0}^{n+1} c_i(f)H_i$, we have $k = 1$ and

$$\begin{aligned}\mathrm{NF}(f) &= \sum_{i=0}^{n-1} c_i(f)H_i + \underline{c_n(f)H_n} + c_{n+1}(f)\,\mathrm{NF}(H_{n+1}) \\ &\equiv \sum_{i=0}^{n-2} c_i(f)H_i + \left(c_{n-1}(f) - nc_{n+1}(f)\right)H_{n-1}\end{aligned}$$

Find $c_i(f)$ as linear combination of the coefficients of f and of H_n.

II. Expectation and normal forms

- Let f be a polynomial in one variable with real coefficients and by polynomial division $f(x) = q(x)H_n(x) + r(x)$ where r has degree smaller than H_n and $r(x) = f(x)$ on $H_n(x) = 0$.
- Then for $Z \sim \mathcal{N}(0,1)$

$$\begin{aligned} \mathrm{E}\,(f(Z)) &= \mathrm{E}\,(q(Z)H_n(Z)) + \mathrm{E}\,(r(Z)) \\ &= \mathrm{E}\,(q(Z)\,\delta^n 1) + \mathrm{E}\,(r(Z)) \\ &= \mathrm{E}\,(d^n q(Z)) + \mathrm{E}\,(r(Z)) = \mathrm{E}\,(r(Z)) \qquad \text{iff } \mathrm{E}(d^n q(Z)) = 0. \end{aligned}$$

- Note that $d^n q(Z) = 0$ if and only if q has degree smaller than n and this is only if f has degree smaller or equal to $2n-1$. But also

$$\mathrm{E}\,(d^n q(Z)) = \mathrm{E}\left(d^n \sum_{i=0}^{\infty} c_i(q)H_i\right) = \langle H_n, \sum_{i=0}^{\infty} c_i(q)H_i\rangle = n!c_n(q) = 0$$

iff $c_n(q) = 0$. The set of polynomials orthogonal to H_n is characterised by $c_n(q) = 0$ which is a linear combination of coefficients of f.

Gaussian quadrature

For $k = 1, \ldots, n$ and $x_1, \ldots, x_n \in \mathbb{R}$ pairwise distinct, define the Lagrange polynomials

$$l_k(x) = \prod_{i:i \neq k} \frac{x - x_i}{x_k - x_i}$$

- These are indicator polynomial functions of degree $n-1$, namely $l_k(x_i) = \delta_{ik}$,
- and form a $\mathbb{R}$-vector space basis of the set of polynomials of degree at most $(n-1)$, $\mathbb{P}_{n-1}$.
- Hence if r has degree smaller than n then $r(x) = \sum_{k=1}^{n} r(x_k) l_k(x)$
- and for $w_k = \mathrm{E}(l_k(Z))$ by linearity

$$\mathrm{E}(r(Z)) = \sum_{k=1}^{n} r(x_k)\,\mathrm{E}(l_k(Z)) = \sum_{k=1}^{n} r(x_k) w_k$$

- Putting all together, on $\mathcal{D}_n = \{x : H_n(x) = 0\} = \{x_1, \dots, x_n\}$ and for f polynomial of degree at most $(2n-1)$ or s.t. $c_n(\frac{f-r}{H_n}) = 0$

$$\begin{aligned} \mathrm{E}\left(f(Z)\right) = \mathrm{E}\left(r(Z)\right) &= \sum_{k=1}^{n} r(x_k)\,\mathrm{E}\left(l_k(Z)\right) \\ &= \sum_{k=1}^{n} f(x_k) w_k \\ &= \mathrm{E_n}\left(f(X)\right) \end{aligned}$$

where $\mathrm{P_n}\left(X = x_k\right) = \mathrm{E}\left(l_k(Z)\right) = w_k$ is a probability on $\mathcal{D}$.

- In general

$$\mathrm{E}\left(f(Z)\right) = \sum_{k=1}^{n} f(x_k)\,\mathrm{E}\left(l_k(Z)\right) + n! c_n\left(\frac{f-r}{H_n}\right)$$

III. Algebraic computation of the weights w_k

Theorem

Let w be the polynomial of degree $n-1$ such that $w(x_k) = w_k$ then

$$w(x)H_{n-1}^2(x) = \frac{(n-1)!}{n} \qquad \text{on } H_n(x) = 0.$$

- E.g. for $n = 3$

$$\begin{cases} 0 &= H_3(x) = x^3 - 3x \\ 2/3 &= w(x)H_2^2 = (\theta_0 + \theta_1 x + \theta_2 x^2)(x^2 - 1)^2 \end{cases}$$

  reduce degree using $x^3 = 3x$ and equate coefficients to obtain

$$w(x) = \frac{2}{3} - \frac{x^2}{6}$$

  Evaluate to find $w_{-\sqrt{3}} = w(-\sqrt{3}) = \frac{1}{6} = w_{\sqrt{3}}$ and $w_0 = w(0) = \frac{2}{3}$.

- The roots of H_n, $n > 2$, are not in $\mathbb{Q}$. Computer algebra systems work with rational fields. Working with algebraic extensions of fields could be slow.
- Sometimes there is no need to compute explicitly the weights.

A CoCoA code for the weighing polynomial

```
N:=4;                                   -- number of nodes
Use R::=Q[w,h[1..(N-1)]], Elim(w);      -- setting up the ring
                                        -- the Hermite polynomials
A:=[ h[I]-h[1]*h[I-1]+(I-1)*h[I-2] | I In (3..(N-1)) ];
Eqs:=Concat( A, [ h[2]-h[1]*h[1]+1 ] );
Append(Eqs,h[1]*h[N-1]-(N-1)*h[N-2]); --the nodes
Set Indentation;
Append(Eqs,N*w*h[N-1]^2-Fact(N-1));    --the weighing polynomial
J:=Ideal(Eqs); GB_J:=GBasis(J);         --the game
Last(GB_J);

3w + 1/4h[2] - 5/4                      --the result
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```

Hence, $w(x) = \frac{5-h[2]}{12} = \frac{6-x^2}{12}$ and as $h[4] = x^4 - 6x^2 + 3 = 0$ we get

x	$-\sqrt{3-\sqrt{6}}$	$-\sqrt{3\pm\sqrt{6}}$	$\sqrt{3-\sqrt{6}}$	$\sqrt{3+\sqrt{6}}$
$w(x)$	$\frac{3+\sqrt{6}}{12}$	$\frac{3-\sqrt{6}}{12}$	$\frac{3+\sqrt{6}}{12}$	$\frac{31\sqrt{6}}{12}$

Proof

- For $\{\tilde{H}_n\}_n$ a sequence of normalised orthogonal polynomials, the Christoffel-Darboux formula recite

$$\sum_{k=0}^{n-1} \tilde{H}_k(x)\tilde{H}_k(t) = \sqrt{\beta_n}\,\frac{\tilde{H}_n(x)\tilde{H}_{n-1}(t) - \tilde{H}_{n-1}(x)\tilde{H}_n(t)}{x-t}$$

$$\sum_{k=0}^{n-1} \tilde{H}_k(t)^2 = \sqrt{\beta_n}\left(\tilde{H}_n'(t)\tilde{H}_{n-1}(t) - \tilde{H}_{n-1}'(t)\tilde{H}_n(t)\right)$$

where $\tilde{H}_{k+1}(t) = (t-\alpha_k)\tilde{H}_k(t) - \beta_k \tilde{H}_{k-1}(t) \qquad \tilde{H}_{-1}(t) = 0 \qquad \tilde{H}_0(t) = 1.$

- For $\tilde{H}_n = H_n/\sqrt{n!}$ and at points in $\mathcal{D}_n = \{x : H_n(x) = 0\}$ they become

$$\sum_{k=0}^{n-1} \tilde{H}_k(x_i)\tilde{H}_k(x_j) = 0 \text{ if } i \neq j \qquad \sum_{k=0}^{n-1} \tilde{H}_k(x_i)^2 = n\tilde{H}_{n-1}(x_i)^2$$

Hence for $\mathbb{H}_n = \left[\tilde{H}_j(x_i)\right]_{i=1,\dots,n;j=0,\dots,n-1}$

$$\mathbb{H}_n\mathbb{H}_n^t = n\, diag(\tilde{H}_{n-1}^2(x_i) : i = 1,\dots,n)$$

and $\mathbb{H}_n^{-1} = \mathbb{H}_n^t n^{-1} diag(\tilde{H}_{n-1}^{-2}(x_i) : i = 1,\dots,n)$.

- Let $f(x) = \sum_{j=0}^{n-1} c_j \tilde{H}_j(x)$ and $\underline{f} = \mathbb{H}_n \underline{c}$ where $\underline{f} = [f(x_i)]_{i=1,\ldots,n}$ and $\underline{c} = [c_j]_j$. Furthermore

$$\begin{aligned} \underline{c} &= \mathbb{H}_n^{-1} \underline{f} = \mathbb{H}_n^t n^{-1} diag(\tilde{H}_{n-1}^{-2}(x_i) : i = 1, \ldots, n) \underline{f} \\ &= \mathbb{H}_n^t n^{-1} diag(\tilde{H}_{n-1}^{-2}(x_i) f(x_i) : i = 1, \ldots, n) \\ c_j &= \frac{1}{n} \sum_{i=1}^{n} \tilde{H}_j(x_i) f(x_i) \tilde{H}_{n-1}^{-2}(x_i) \end{aligned}$$

- For $f(x) = l_k(x)$ the kth Lagrange polynomial and using $l_k(x_i) = \delta_{ik}$ above

$$c_j = \frac{1}{n} \tilde{H}_j(x_k) \tilde{H}_{n-1}^{-2}(x_k)$$

- The expected value of $l_k(Z)$ is

$$w_k = \mathrm{E}\left(l_k(Z)\right) = \sum_{j=0}^{n-1} c_j \, \mathrm{E}\left(\tilde{H}_j(x)\right) = c_0 = \frac{1}{n} \tilde{H}_{n-1}^{-2}(x_k)$$

IV. Fractions: $\mathcal{F} \subset \mathcal{D}_n$, $\#\mathcal{F} = m < n$

- Let $1_{\mathcal{F}}(x)$ be the polynomial of degree n such that $1_{\mathcal{F}}(x) = 1$ if $x \in \mathcal{F}$ and 0 if $x \in \mathcal{D}_n \setminus \mathcal{F}$ and

  let f be polynomial of degree at most $n-1$ or s.t. $c_n((f1_{\mathcal{F}} - r)/H_n) = 0$ and

  let $Z \sim \mathcal{N}(0,1)$.

  Then

$$\mathrm{E}((f1_{\mathcal{F}})(Z)) = \sum_{x_k \in \mathcal{F}} f(x_k)w_k = \mathrm{E_n}\left(f(X)1_{\mathcal{F}}(X)\right)$$
$$= \mathrm{E_n}\left(f(X)|X \in \mathcal{F}\right)\mathrm{P_n}(X \in \mathcal{F})$$

  where $\mathrm{P_n}(X = x_k) = w_k$.

- Let $\omega_{\mathcal{F}}(x) = \prod_{x_k \in \mathcal{F}} (x - x_k) = \sum_{i=0}^{m} c_i H_i(x)$[1] and note $l_k^{\mathcal{F}}(x) = \prod_{i \in \mathcal{F}, i \neq k} \frac{x - x_i}{x_k - x_i} = \mathrm{NF}(l_k(x), \mathrm{Ideal}(\omega_{\mathcal{F}}(x))$ are the Lagrange polynomials for $\mathcal{F}$.

  Let f be a polynomial of degree N and $f(x) = q(x)\omega_{\mathcal{F}}(x) + r(x)$ with $f(x_i) = r(x_i)$ on $\mathcal{F}$ and $r(x) = \sum_{x_k \in \mathcal{F}} f(x_k) l_k^{\mathcal{F}}(x)$.

  Let's write $q(x) = \sum_{j=0}^{N-m} b_j H_j(x)$.

  Then

$$\mathrm{E}\left(f(Z)\right) = \mathrm{E}\left(\sum_{j=0}^{N-m} b_j H_j(Z) \sum_{i=0}^{m} c_i H_i(Z)\right) + \mathrm{E}\left(r(Z)\right)$$

$$= b_0 c_0 + b_1 c_1 + \ldots + ((N-m) \wedge m)! \, b_{(N-m)\wedge m} c_{(N-m)\wedge m} + \sum_{x_k \in \mathcal{F}} f(x_k) w_k^{\mathcal{F}}$$

  where $w_k^{\mathcal{F}} = \mathrm{E}\left(\mathrm{NF}(l_k(x), \mathrm{Ideal}(\omega_{\mathcal{F}}(x)))\right)$.

[1] cf. the node polynomial from Gautschi.

V. Higher dimension

Theorem (Full grid on the zeros of product of Hermite polynomials)

Let $Z_1, \ldots, Z_d$ *i.i.d.* $\sim \mathcal{N}(0,1)$, $f \in \mathbb{R}[x_1, \ldots, x_d]$ *with* $\deg_{x_i} f \leq 2n_i - 1$ *for* $i = 1, \ldots, d$ *and*

$$\mathcal{D}_{n_1 \ldots n_d} = \{(x_1, \ldots, x_d) \in \mathbb{R}^d : H_{n_1}(x_1) = H_{n_2}(x_2) = \ldots = H_{n_d}(x_d) = 0\}.$$

Then

$$\mathrm{E}\left(f(Z_1, \ldots, Z_d)\right) = \sum_{(x_1, \ldots, x_d) \in \mathcal{D}_{n_1 \ldots n_d}} f(x_1, \ldots, x_d) w_{x_1}^{n_1} \ldots w_{x_d}^{n_d}$$

where $w_{x_j}^{n_j} = \mathrm{E}\left(l_{x_j}(Z_j)\right)$ *for* $x_j \in \mathcal{D}_{n_j}$.

- Here $\mathrm{E}\left(f(Z_1, Z_2)\right) = \int f(x, y) \frac{e^{-(x^2+y^2)/2}}{\sqrt{2\pi}^2} dxdy$
- Can take other f e.g. for $f(x,y) = q_1(x,y)H_n(x) + q_2(x,y)H_m(y) + r(x,y)$ is needed that $\mathrm{E}\left(d_x^n q_1(Z_1, Z_2)\right)$ and $\langle H_m(Z_2), q_2(Z_1, Z_2)\rangle = 0$.
- For Z_1 and Z_2 dependent with known covariance then without changing degrees the previous applies.

Fraction: an example

- $$\begin{cases} g_1 = x^2 - y^2 & = H_2(x) - H_2(y) = 0 \\ g_2 = y^3 - 3y & = H_3(y) = 0 \\ g_3 = xy^2 - 3x & = H_1(x)\left(H_2(y) - 2H_0\right) = 0 \end{cases}$$
- For any f polynomial there exists unique $r \in \text{Span}\left(1, x, y, xy, y^2\right) = \text{Span}\left(H_0, H_1(x), H_1(y), H_1(x)H_1(y), H_2(y)\right)$ such that $f = \sum_{i=1}^{3} q_i g_i + r$.
- If

$$\begin{aligned} q_1(x,y) &= a_o + a_1 H_1(x) + a_2 H_1(y) + a_3 H_1(x) H_1(y) \\ q_2(x,y) &= \theta_1(x) + \theta_2(x) H_1(y) + \theta_3(x) H_2(y) \\ q_3(x,y) &= a_4 + a_5 H_1(y) \end{aligned}$$

- Then

$$\begin{aligned} \mathrm{E}(f(Z_1, Z_2)) &= \mathrm{E}(r(Z_1, Z_2)) \\ &= 2\frac{f(0,0)}{3} + \frac{f(\sqrt{3},\sqrt{3}) + f(\sqrt{3},-\sqrt{3}) + f(-\sqrt{3},\sqrt{3}) + f(-\sqrt{3},-\sqrt{3})}{12} \end{aligned}$$

Input: $\mathcal{F} \subset \{(x_1, \ldots, x_d) : H_{n_i}(x_i) = 0 \; i = 1, \ldots, d\}$
τ and f polynomial
Output: $\mathrm{E}(f(Z))$ with $Z \sim \mathcal{N}_n(0, I)$

1. Compute G, a τ-Gröbner basis of the design ideal of $\mathcal{F}$
2. Let $H = \{h = h_{a_1}(x_1) \ldots h_{a_d}(x_d) : \mathrm{LT}_\tau(h) \leq_\tau \mathrm{LT}_\tau(g) \text{ for all } g \in G\}$
(the Hermite basis of the linear space of monomials in the g's)
3. Write $g \in G$ in terms of Hermite polynomials
(change of linear basis from "monomials" to "Hermite")
4. Write $f = \sum_{g \in G} s_g g + r = \sum_{g \in G} s_g \sum_{h<g} g_h h + r$
5. Check if $\sum_{g \in G, h<g} \langle s_g g_h, h \rangle = 0$ for all $h = h_{a_1}(x_1) \ldots h_{a_d}(x_d) \in H$
(more often than not complicated linear combination of coefficients of f)
6. If YES then $\mathrm{E}(f(Z)) = \sum_{x \in \mathcal{F}} f(x) w_x$
7. If NO then $\mathrm{E}(f(Z)) = \sum_{x \in \mathcal{F}} f(x) w_x +$ complicated linear combination of coefficients of f

Notes:

- 1., 2., 3. and 4. are essentially linear operations.
- Find $\mathcal{F}$ and f such that 5. holds.
- By means of a Buchberger-Möller type of algorithm do 1.2.3. directly with Hermite polynomials. What about 4. and 5.? We think we have 7.

Factorial grid

Design

$$\mathcal{G} = \begin{cases} g_1 = y(y-1) & = H_2(y) - H_1(y) + 1 \\ g_2 = x(x-1)(x-2) & = H_3(x) - 3H_2(x) + 5H_1(x) - 3H_0(x) \end{cases}$$

Then the only order ideal is

$$\begin{aligned} \mathcal{L} &= \{1, y, x, xy, x^2, x^2y\} \\ &= \{H_0, H_1(y), H_1(x), H_1(y)H_1(x), H_2(x)+1, H_2(x)H_1(x)+H_1(x)\} \end{aligned}$$

and $f \in \mathbb{R}[x, y]$ can be written as $f = s_1 g_1 + s_2 g_2 + r$ with $r \in \operatorname{Span} \mathcal{L}$. Then

$$\begin{aligned} \mathrm{E}(f(X,Y)) = &\, \mathrm{E}(s_1(H_2(Y) - H_1(Y) + 1)) \\ &+ \mathrm{E}(s_2(H_3(X) - 3H_2(X) + 5H_1(X) - 3H_0(X)) + \mathrm{E}(R) \end{aligned}$$

As $s_1 = \sum_{i,j=0}^{+\infty} \alpha_{ij} H_i(x) H_j(y)$ with only a finite number of $\alpha_{ij} \in \mathbb{R}$ not zero, we have

$$\begin{aligned}
\mathrm{E}(s_1(H_2(Y) - H_1(Y) + 1)) &= \sum_{i,j=0}^{+\infty} \alpha_{ij} \int H_i(x)dx \int H_j(y)H_2(y)dy \\
&- \sum_{i,j=0}^{+\infty} \alpha_{ij}(\int H_i(x)dx \int H_j(y)H_1(y)dy) \\
&+ \sum_{i,j=0}^{+\infty} \alpha_{ij}(\int H_i(x)dx \int H_j(y)dy) \\
&= \sum_{i,j=0}^{+\infty} \alpha_{ij}\delta_{i,0}2!\delta_{j,2} - \sum \alpha_{ij}\delta_{i,0}1!\delta_{j,1} + \sum \alpha_{ij}\delta_{i,0}0!\delta_{j,0} \\
&= 2!\alpha_{0,2} - \alpha_{0,1} + \alpha_{0,0} \qquad (1)
\end{aligned}$$

Similarly for $g_2 = H_3(x) - 3H_2(x) + 5H_1(x) - 3H_0(x)$ and $s_2 = \sum_{i,j=0}^{+\infty} \beta_{ij} H_i(x) H_j(y)$ we find

$$\mathrm{E}(s_2 g_1) = 3!\beta_{3,0} - 3 \cdot 2!\beta_{2,0} + 5\beta_{1,0} - 3\beta_{0,0} \qquad (2)$$

For any f orthogonal to g_1 and g_2, that is, such that

$$2!\alpha_{0,2} - \alpha_{0,1} + \alpha_{0,0} = 0 = 3!\beta_{3,0} - 3 \cdot 2!\beta_{2,0} + 5\beta_{1,0} - 3\beta_{0,0}$$

$$\mathrm{E}(f(X,Y)) = \sum_{d \in \mathcal{D}} f(d)\,\mathrm{E}(w_d(X,Y))$$

where e.g. $w_d(x,y)$ is the product of the Lagrange polynomial for the levels of x and the Lagrange polynomial for the levels of y.

- The steps in magenta require only linear algebra operation and involve only the H's.
- The green bits, the s_i may not be unique.
- The red bits, what we care about, can be determined easily. The issues are to find how they relate to the coefficients of f and how the non-uniqueness of s_i effects them.

We think that the above can be generalised

- to any product grid with integer levels, and likely for any level,
- to other types of design e.g. we considered $(x, x^2) : x = -2, -1, 0, 1, 2.$

  The G-Bases and the quotient space bases can be obtained by a specialisation of the Buchberger Möller algorithm for ideal of points.

  Even if the s_i's are not unique, we suspect that there is some invariants (simpler than sizygies).

  In any case we still need to write the "Hermite coefficients" in terms of the coefficients of the polynomial to integrate.

Of course we'd like to implement efficient macros.

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Product formula

Let $\langle \phi, \psi \rangle = \mathrm{E}(\phi(Z)\psi(Z))$ and $h < k$. Then

$$\langle H_k H_h, \psi \rangle = \langle H_h, H_k \psi \rangle = \langle 1, d^h(H_k\psi) \rangle = \sum_{i=0}^{h} \langle 1, \binom{h}{i} d^i H_k d^{h-i} \psi \rangle$$

$$= \langle 1, H_k d^h \psi \rangle + \sum_{i=1}^{h} \langle 1, \binom{h}{i} d^i H_k d^{h-i} \psi \rangle$$

$$= \langle H_{h+k}, \psi \rangle + \sum_{i=1}^{h} \binom{h}{i} k(k-1)\ldots(k-i+1) \langle H_{h+k-2i}, \psi \rangle$$

Example: $H_2 H_1 = (x^2 - 1)x = H_3 + 2H_1$ and in particular

$$H_k^2 = H_{2k} + \sum_{i=1}^{k} \binom{k}{i} k(k-1)\ldots(k-i+1) H_{2k-2i}$$

$$\mathrm{E}(H_k^2(Z)) = \binom{k}{1} k(k-1)\ldots 1 = k!$$

$$\mathrm{E}(H_k(Z) H_h(Z)) = 0$$

Algebraic DoE: basics

- Given a finite set $\mathcal{D}$ of distinct points in $\mathbb{R}^d$ we consider the design ideal

$$\begin{aligned}&\langle f \in \mathbb{R}[x_1, \ldots, x_d] : f(d) = 0 \text{ for all } d \in \mathcal{D}\rangle \\ =&\langle f_1, \ldots, f_p \in \mathbb{R}[x_1, \ldots, x_d]\rangle\end{aligned}$$

- Two polynomials h, k, are aliased if $h - k$ is zero on $\mathcal{D}$, i.e. if $h - k$ belong to the design ideal.
- A fraction is a subset $\mathcal{F}$ of $\mathcal{D}$. Its design ideal is obtained by adding new equations $g_1, \ldots, g_l$, called defining equations.
- The indicator polynomial of the fraction $\mathcal{F}$ in $\mathcal{D}$ is a polynomial whose restriction to $\mathcal{D}$ is the indicator function of the fraction.
- This is made operative by notions from Algebraic Geometry such as term-order, Gröbner basis, normal form, ... and algebraic software such as CoCoA, Maple, Singular, `4ti2`, Matematica, Maxima, Macaulay2, ...

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An application: identification of Fourier coefficients in one dimension

For $f(x) = \sum_{k=0}^{N} c_k(f) H_k(x)$, then

- $\mathrm{E}(f(Z)) = c_0(f)$
- if $c_n((f-r)/H_n) = 0$ e.g. if $N \leq 2n-1$ then
$$c_0(f) = \sum_{H_n(x_k)=0} f(x_k) w_k.$$
- If $c_n((f\,H_i - r)/H_n) = 0$ e.g. for all i such that $N + i \leq 2n - 1$
$$\sum_{H_n(x_k)=0} f(x_k) H_i(x_k) w_k = \mathrm{E}(f(Z) H_i(Z)) = i! c_i(f),$$
- in particular if $\deg f = n-1$ then all coefficients can be computed exactly.
- In general
$$\sum_{H_n(x_k)=0} f(x_k) H_i(x_k) w_k = \sum_{H_n(x_k)=0} \mathrm{NF}(f(x_k) H_i(x_k)) w_k$$
$$= \mathrm{E}(\mathrm{NF}(f(Z) H_i(Z))) = i! c_i(\mathrm{NF}(f)).$$

...in higher dimension

Consider $\mathcal{D}_{nn}$ and f a polynomial with $\deg_x f, \deg_y f < n$ then

$$f(x, y) = \sum_{i,j=0}^{n-1} c_{ij} H_i(x) H_j(y)$$

As $\deg_x(fH_k), \deg_y(fH_k) < 2n - 1$ for all $k < n$, then

$$\begin{aligned} \mathrm{E}\left(f(Z_1, Z_2)H_k(Z_1)H_h(Z_2)\right) &= c_{hk}\delta_{ik}||H_k(Z_1)||^2\delta_{jh}||H_h(Z_2)||^2 \\ c_{kh} &= \frac{1}{k!h!} \sum_{(x,y)\in\mathcal{D}_{nn}} f(x, y)H_k(x)H_h(y)w_x w_y \end{aligned}$$

Note if f is the indicator function of a fraction $\mathcal{F} \subset \mathcal{D}_{nn}$ then

$$c_{kh} = \frac{1}{k!h!} \sum_{(x,y)\in\mathcal{F}} H_k(x)H_h(y)w_x w_y$$