WOGAS2

Hermite polynomial aliasing in Gaussian quadrature

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A representation of some Hermite polynomials, including those of degree $2n-1$, as sum of an element in the polynomial ideal generated by the roots of the Hermite polynomial of degree n and of a reminder, suggests a folding of multivariate polynomials over a finite set of points. From this, the expectation of some polynomial combinations of random variables normally distributed is computed. This is related to quadrature formulas and has strong links with designs of experiments.

I. Stein-Markov operator for standard normal distribution

Define $\delta f(x) = xf(x) - f'(x) = -e^{x^2/2} \frac{d}{dx} \left(f(x) e^{-x^2/2} \right)$

and let $Z \sim \mathcal{N}(0,1)$ and $d^n = \frac{d^n}{dx^n}$. Then

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

For conditions on g, f see Malliavin V Lemma 1.3.2 and Proposition 2.2.3. Polynomials satisfy these conditions.

1. $H_n(x) = \delta^n 1$, the monic Hermite polynomial of degree n

$$H_0 = 1 \quad H_1(x) = x \quad H_2(x) = x^2 - 1 \quad H_3(x) = x^3 - 3x$$

2. $d\delta - \delta d = id$ and $dH_n = nH_{n-1}$ and $H_{n+1} = xH_n - nH_{n-1}$
3. The formula shows that the H_n's are orthogonal

Ring structure of Hermite polynomials

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

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

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

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

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

Exercise: $H_2 H_1 = (x^2 - 1)x = H_3 + 2H_1$ $\qquad H_k^2 = H_{2k} + \sum_{i=1}^{k} \binom{k}{i}^2 i! H_{2k-2i}$

$$\mathrm{E}(H_k^2(Z)) = \binom{k}{1} k(k-1)\dots 1 = k! \qquad \mathrm{E}(H_k(Z) H_h(Z)) = 0$$

An exercise

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 $r(x) = f(x)$ if $H_n(x) = 0$. The $n-1$ degree polynomial r is fundamental and is referred to as reminder or normal form. Then

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

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

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

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

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 $n-1$, $\mathbb{P}_{n-1}$. Namely if r has degree smaller than n then $r(x) = \sum_{k=1}^n r(x_k) l_k(x)$ and for $\lambda_k = \mathrm{E}(l_k(Z))$ by linearity $\mathrm{E}(r(Z)) = \sum_{k=1}^n r(x_k)\,\mathrm{E}(l_k(Z)) = \sum_{k=1}^n r(x_k)\lambda_k$.

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

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

where $\mathrm{P_n}\left(X = x_k\right) = \mathrm{E}\left(l_k(Z)\right) = \lambda_k$, cf. standard results on Gaussian quadrature (Gautschi Chapter 1).

Applications: 1) identification

Let $f(x) = \sum_{k=0}^{N} c_k(f) H_k(x)$, then if $N \le 2n - 1$

$$\sum_{H_n(x_k)=0} f(x_k)\lambda_k = \mathrm{E}(f(Z)) = c_0(f)$$

for all i s.t. $N + i \le 2n - 1$

$$\sum_{H_n(x_k)=0} f(x_k) H_i(x_k)\lambda_k = \mathrm{E}(f(Z)H_i(Z)) = i!\, c_i(f)$$

e.g. $\deg f = n - 1$ then all coefficients can be computed exactly.
In general

$$\sum_{H_n(x_k)=0} f(x_k) H_i(x_k)\lambda_k = \sum_{H_n(x_k)=0} \mathrm{NF}(f(x_k)H_i(x_k))\lambda_k$$
$$= \mathrm{E}(\mathrm{NF}(f(Z)H_i(Z))) = i!\, c_i(\mathrm{NF}(f))$$

and 2) confounding

The computation of the normal form introduces a notion of confounding. For example from $H_{n+1}(x) = xH_n(x) - nH_{n-1}(x)$ and for $\equiv$ meaning equality holds over $\mathcal{D}_n = \{x : H_n(x) = 0\}$, easilly $H_{n+1}(x) \equiv -nH_{n-1}(x)$ follows. In general let $H_{n+k} \equiv \sum_{j=0}^{n-1} h_j^{n+k} H_j$ be the Fourier expansion of H_{n+k} at $\mathcal{D}_n$. Substituting 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

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

and all coefficients up to degree $n-2$ are clean.

II. Algebraic computation of the weights λ_k

Orthogonal monic polynomials satisfy three-term-recurrence relation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t) \qquad \pi_{-1}(t) = 0 \qquad \pi_0(t) = 1$$

with $\alpha_k = \dfrac{\langle t\pi_k, \pi_k \rangle}{\langle \pi_k, \pi_k \rangle}$ and $\beta_k = \dfrac{\langle \pi_k, \pi_k \rangle}{\langle \pi_{k-1}, \pi_{k-1} \rangle}$. Note $||\pi_n||^2 = \beta_n \beta_{n-1} \dots \beta_0$
For the orthonormal polynomials the Christoffel-Darboux formula hold

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

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

For Hermite polynomials $\alpha_n = 0$, $\beta_n = n$, $\tilde{H}_n(x) = H_n(x)/\sqrt{n!}$ and $\tilde{H}'_n(x) = \sqrt{n}\tilde{H}_{n-1}(x)$. Substituting above for x_i: $H_n(x_i) = 0$ gives

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

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

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

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

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

Apply to $f(x) = l_k(x) = \sum_{j=0}^{n-1} c_{kj}\tilde{H}_j(x)$ the kth Lagrange polynomial

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

using $l_k(x_i) = \delta_{ik}$ in (1).

The expected value of $l_k(Z)$ is

$$\lambda_k = \mathrm{E}\left(l_k(Z)\right) = \sum_{j=0}^{n-1} c_{kj}\,\mathrm{E}\left(\tilde{H}_j(x)\right) = c_{k0}$$

We have proved

Theorem

The weights λ_k, $k = 1, \ldots, n$ are

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

Let l be the polynomial of degree $n-1$ such that $l(x_k) = \lambda_k$ then

$$\left\{ \begin{array}{ll} H_n(x) = 0 & H_n(x) = 0 \\ l(x)\tilde{H}_{n-1}^2(x) = n^{-1} & l(x)H_{n-1}^2(x) = \dfrac{(n-1)!}{n} \end{array} \right\}$$

Notes

- Compute $\mathrm{E}(l_k(Z))$ once for all
- e.g. for $n = 3$

$$0 = H_3(x) = x^3 - 3x$$
$$2/3 = l(x)H_2^2 = (\theta_0 + \theta_1 x + \theta_2 x^2)(x^2 - 1)^2$$

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

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

  Evaluate to find $\lambda_{-\sqrt{3}} = l(-\sqrt{3}) = \frac{1}{6} = \lambda_{\sqrt{3}}$ and $\lambda_0 = l(0) = \frac{2}{3}$.
- The case $n = 4$ shows that the λ_k can be not rational numbers.
- $p - l(x)$ is the interpolating polynomials of the set of points $\{(\lambda_k, x_k), k = 1, \ldots, n\}$.
- The roots of H_n are real but usually not rational numbers. Computer algebra systems works with integer or rational fields. Working with algebraic extensions of fields could be slow.
- Sometimes there is no need to compute explicitly the weights.

Theorem

Let $f(x)$ be a polynomial and $f(x) = q(x)H_n(x) + r(x)$ where q, r are unique with r of degree less than n. Let $Z \sim \mathcal{N}(0,1)$. Then $f - qH_n$ is the unique polynomial in $\mathbb{P}_{n-1}$ such that for all $m \geq n$

$$\mathrm{E}\left((f(Z) - q(Z)H_n(Z))H_m(Z)\right) = 0$$

Proof.

- r has degree at most $n-1$, then $r(x) \in \mathrm{Span}(H_1, \ldots, H_{n-1})$. In particular r is orthogonal to H_m for all $m \geq n$.
- Let there exist q_1 and q_2 distinct such that $f - q_1 H_n \perp H_m$ and $f - q_2 H_n \perp H_m$ for all $m \geq n$. Now $(q_1 - q_2)H_n$ is 0 or has degree not smaller than n. Furthermore it is orthogonal to H_m for all $m \geq n$. Necessarily it is 0, equivalently $q_1 = q_2$.

□

From $q = \sum_{j \geq 0} c_j(q) H_j$ and $\mathrm{E}\left((f - \sum_{j\geq 0} c_j(q) H_j H_n) H_m\right) = 0$ for all $m \geq n$ get $c_m(f)/m! = \sum_{j \geq 0} c_j(q)\,\mathrm{E}\left(H_j H_n H_m\right)$ which can be simplified by e.g. using the product formula.

III. 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 $n-1$ and let $Z \sim \mathcal{N}(0,1)$. Then for $\mathrm{P_n}(X = x_k) = \lambda_k$

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

• Let $\omega_{\mathcal{F}}(x) = \prod_{x_k \in \mathcal{F}} (x - x_k) = \sum_{i=0}^{m} c_i H_i(x)$ 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 $\mathcal{F}$. For f a polynomial of degree N, wite $f(x) = q(x)\omega_{\mathcal{F}}(x) + r(x)$ 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 $q(x) = \sum_{j=0}^{N-m} b_j H_j(x)$. Then

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

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

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

IV. Higher dimension

Theorem

Let $Z_1, \dots, Z_d$ *i.i.d.* $\sim \mathcal{N}(0,1)$, $f \in \mathbb{R}[x_1, \dots, x_d]$ *with* $\deg_{x_i} f \leq 2n_i - 1$ *for* $i = 1, \dots, d$ *and*
$\mathcal{D}_{n_1 \dots n_d} = \{x = (x_1, \dots, x_d) \in \mathbb{R}^d : H_{n_1}(x_1) = H_{n_2}(x_2) = \dots = H_{n_d}(x_d) = 0\}$.
Then

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

Exercise: let $\mathcal{F}$ be the zero set of

$$\begin{cases} g_1 = x^2 - y^2 & = H_2(x) - H_2(y) = 0 \\ g_2 = y^3 - 3y & = H_3(y) = 0 \\ g_3 = xy^2 - 3x & = H_1(x)\left(H_2(y) - 2H_0\right) = 0 \end{cases}$$

For f polynomial there exists unique
$r \in \mathrm{Span}\left(H_0, H_1(x), H_1(y), H_1(x)H_1(y), H_2(y)\right) = \mathrm{Span}\left(1, x, y, xy, y^2\right)$ s.t.
$f = \sum q_i g_i + r$. If $q_1(x,y) = a_o + a_1 H_1(x) + a_2 H_1(y) + a_3 H_1(x) H_1(y)$,
$q_2 = \theta_1(x) + \theta_2(x) H_1(y) + \theta_3(x) H_2(y)$, $q_3 = a_4 + a_5 H_1(y)$ then

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

An application

Let f be a polynomial with $\deg_x f, \deg_y f < n$ and consider $\mathcal{D}_{nn}$ 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

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

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

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

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