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A General Expression for Hermite Expansions with Applications

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ABSTRACT: Hermite polynomials arise when dealing with functions of normally distributed variables, and are commonly thought of as the analog of the simple polynomials on functions of regular variables. Therefore the Hermite expansion should be an analog of the Taylor expansion. Indeed there is a strong connection between the two – the general coefficient in the Hermite expansion is the weighted integral of the n^{th} derivative, as compared to the n^{th} derivative evaluated at zero in the case of Taylor. This fact can be used to derive the Hermite expansion for the integral and the derivative of a function. Furthermore, it provides a method of providing simple proofs of many of the Hermite identities. This connection is used to derive the Hermite expansions of the normal probability distribution function, the normal cumulative distribution function and the indicator function. Finally, an algorithm to numerically perform a Hermite expansion is presented, which is efficient in the sense that is only requires a single call to a quadrature method.

Keywords: Hermite polynomials, Hermite expansion, Gauss-Hermite quadrature

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Introduction

The Hermite polynomials are a ubiquitous set of orthogonal polynomials (see, for instance [1, 2]) that appear wherever a Gaussian distribution is used, and thus naturally arise in many disciplines such as physics (e.g. quantum harmonic oscillator), statistics (e.g. Gram-Charlier Type A and Edgeworth expansions, Hermite series estimators and sequential Hermite series estimators) and finance (e.g. option pricing). Hermite polynomials are defined by the Rodrigues formula [9]

$$H_n(x) = \frac{(-1)^n}{\omega(x)} \frac{\partial^n}{\partial x^n} \omega(x), \tag{0.1}$$

with the Gaussian weighting function

$$\omega(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{x^2}{2}\right). \tag{0.2}$$

As the Hermite polynomials form a complete basis of polynomials, any polynomial of degree m can be written in the Hermite basis

$$p_m(x) = \sum_{n=0}^{m} d_n H_n(x). \tag{0.3}$$

Furthermore, they can be used to approximate any $L_2(\mathbb{R}, \omega(x)dx)$ function via the Hermite expansion

$$f(x) = \sum_{n=0}^{\infty} d_n H_n(x) \tag{0.4}$$

since the Hermite polynomials are an orthogonal basis for $L_2(\mathbb{R}, \omega(x)dx)$ where the coefficients can be calculated by orthogonality

$$d_n = \frac{1}{n!} \int_{-\infty}^{\infty} f(x) H_n(x) \omega(x) dx. \tag{0.5}$$

In this paper, a general expression for the coefficients d_n is presented, which can be used to easily calculate Hermite identities. In the light of this expression, derivatives and integrals of Hermite expansions take on a simple form, reminiscent of Ito integrals and Malliavin derivatives of the Weiner chaos expansion [6, 4].

This expression can be used to find simple and novel proofs of the following Hermite identities:

- The generating function of a normally distributed variable – Theorem 2.1
- The Hermite inversion theorem – Theorem 2.2
- The three term Hermite recurrence relation – Theorem 2.3
- The Hermite multiplication theorem – Theorem 2.4
- A Hermite convolution integral – Theorem 2.7
- A novel proof of the Hermite linearization theorem – Theorem 2.8

Subsequently, the Hermite expansions are calculated for functions of interest:

- The probability distribution function of a $\mathcal{N}(0, \sigma^2)$ distributed variable – Theorem 2.9
- The cumulative distribution function – Theorem 2.10
- The indicator function – Theorem 2.11

Although these identities are all known, this approach provides alternative, and simpler, proofs. For example, Kagawa calculates the the Hermite coefficients for the indicator function by direct integration [7], and in Chihara et. al. calculate the same by means of a Bargmann transform [3]. The proof in this paper does not rely on the detailed analysis present in the earlier proofs.

Finally, an algorithm for computing the coefficients using Gauss-Hermite quadrature (GHQ) is presented, where these coefficients arise naturally. In particular, the algorithm is efficient, since it only requires a single call to N^{th} order GHQ, from which all d_n can be calculated for $n \in \{0, N-1\}$, with accuracy decreasing as n increases. In order to precisely define the accuracy, an analysis of the error of this algorithm is performed.

1 A General Expression for the Coefficients of a Hermite Expansion

Theorem 1.1. *Given a function $f(x) \in L_2(\mathbb{R}, \omega(x)dx)$ that is square integrable with respect to the Gaussian weighting function*

$$\int_{-\infty}^{\infty} |f(x)|^2 \omega(x) dx < \infty, \tag{1.1}$$

and further

$$\lim_{x \to \pm\infty} f(x)\omega(x) = 0, \tag{1.2}$$

then the coefficients of the Hermite polynomial expansion

$$f(x) = \sum_{n=0}^{M} d_n H_n(x) \tag{1.3}$$

are given by the weighted integral of the n^{th} derivative of $f(x)$

$$d_n = \frac{1}{n!} \int_{-\infty}^{\infty} \frac{\partial^n f(x)}{\partial x^n} \omega(x) dx. \tag{1.4}$$

The constant M can be an integer or infinite.

Proof. The n^{th} coefficient in the Hermite expansion is given by Equation (0.5)

$$d_n = \frac{1}{n!} \int_{-\infty}^{\infty} f(x) H_n(x) \omega(x) dx, \tag{1.5}$$

which, by definition of Hermite polynomials in Equation (0.1), can be written

$$d_n = \frac{1}{n!} \int_{-\infty}^{\infty} f(x) (-1)^n \frac{\partial^n}{\partial x^n} \omega(x) dx. \tag{1.6}$$

By assumption, the function $f(x)$ is square integrable and the product of it and the Gaussian weighting function vanishes at infinity. Therefore (1.6) can be integrated by parts n times to obtain the expression in Equation (1.4). □

Just as the coefficients of a Taylor expansion are the derivatives of the function evaluated at zero, the coefficients of the Hermite polynomial expansion are also related to the derivatives – they are the weighted integrals of the derivatives over the entire real line.

Unfortunately this method is not generalizable to other sets of orthogonal polynomials, since it relies on the simple structure of the Hermite Rodrigues formula (0.1). The general form of the Rodrigues formula is

$$P_n(x) = \frac{a_n}{\omega(x)} \frac{\partial^n}{\partial x^n} \left[(B(x))^n \omega(x) \right], \tag{1.7}$$

and the integration by parts relies on the fact that $B(x) = 1$ which is only true for the Gaussian weighting function.

Theorem 1.2. *Given a function $f(x) \in \mathcal{C}^{(M)}$ that obeys the same integrability conditions as in Theorem 1.1 and has coefficients of a Hermite expansion d_n, then the Hermite expansion of the derivative is given by*

$$\frac{\partial f(x)}{\partial x} = \sum_{n=0}^{M-1} (n+1) d_{n+1} H_n(x). \tag{1.8}$$

Proof. The derivative $\frac{\partial f(x)}{\partial x}$ has a Hermite expansion

$$\frac{\partial f(x)}{\partial x} = \sum_{n=0}^{M-1} c_n H_n(x), \tag{1.9}$$

with n^{th} term

$$c_n = \frac{1}{n!} \int_{-\infty}^{\infty} \frac{\partial^{n+1} f(x)}{\partial x^{n+1}} \omega(x) dx. \tag{1.10}$$

Compare this to the $(n+1)^{\text{st}}$ term in the Hermite expansion for $f(x)$

$$d_{n+1} = \frac{1}{(n+1)!} \int_{-\infty}^{\infty} \frac{\partial^{n+1} f(x)}{\partial x^{n+1}} \omega(x) dx \tag{1.11}$$

demonstrates that $c_n = (n+1)d_{n+1}$, resulting in Equation (1.8). □

Theorem 1.3. *Given a function $f(x) \in \mathcal{C}^{(M)}$ that obeys the same integrability conditions as in Theorem 1.1 and has coefficients of a Hermite expansion d_n, then the Hermite expansion of its anti-derivative $F(x)$ defined by*

$$\int_C^x f(y) dy = F(x) \tag{1.12}$$

is

$$F(x) = b_0 + \sum_{n=1}^{M+1} \frac{1}{n} d_{n-1} H_n(x), \tag{1.13}$$

where $b_0 = \int_{-\infty}^{\infty} F(x)\omega(x)dx$ and C is some (possibly infinite) constant.

Proof. The function $F(x)$ has a Hermite expansion

$$F(x) = \sum_{n=0}^{M+1} b_n H_n(x) \tag{1.14}$$

where the $n = 0$ term is given by

$$b_0 = \int_{-\infty}^{\infty} F(x)\omega(x)dx \tag{1.15}$$

and subsequent terms are given by

$$b_n = \frac{1}{n!} \int_{-\infty}^{\infty} \frac{\partial^{n-1} f(x)}{\partial x^{n-1}} \omega(x) dx \tag{1.16}$$

where $\frac{\partial^0 f(x)}{\partial x^0} = f(x)$ has been used. Compare this to the $(n-1)^{\text{st}}$ term in the Hermite expansion for $f(x)$

$$d_{n-1} = \frac{1}{(n-1)!} \int_{-\infty}^{\infty} \frac{\partial^{n-1} f(x)}{\partial x^{n-1}} \omega(x) dx \tag{1.17}$$

demonstrates that $b_n = \frac{1}{n} d_{n-1}$, resulting in Equation (1.13). □

2 Applications

2.1 Hermite Identities

Hermite identities have very simple proofs as a result of Theorem 1.1.

Theorem 2.1 (Generating function of the normal distribution). *The generating function for the normal distribution is given by*

$$e^{xt-\frac{1}{2}t^2} = \sum_{n=0}^{\infty} \frac{t^n}{n!} H_n(x). \tag{2.1}$$

Proof. Take $f(x) = e^{xt}$. The n^{th} order coefficient of the Hermite expansion is given by

$$\begin{aligned} d_n &= \frac{t^n}{n!} \int_{-\infty}^{\infty} e^{xt} \omega(x) dx &(2.2)\\ &= e^{\frac{1}{2}t^2} \frac{t^n}{n!} &(2.3) \end{aligned}$$

leading to the Hermite expansion that is exactly Equation (2.1). □

Theorem 2.2 (Hermite inversion Theorem). *The polynomials have an expansion in terms of Hermite polynomials given by*

$$x^m = m! \sum_{k=0}^{\lfloor \frac{m}{2} \rfloor} \frac{1}{2^k k!(m-2k)!} H_{m-2k}(x). \tag{2.4}$$

Proof. Take $f(x) = x^m$. The n^{th} coefficient of the Hermite expansion is given by

$$\begin{aligned} d_n &= \frac{1}{n!} \int_{-\infty}^{\infty} \frac{\partial^n}{\partial x^n} x^m \omega(x) dx &(2.5)\\ &= \begin{cases} \binom{m}{n}(m-n-1)!! & m-n \text{ even} \\ 0 & m-n \text{ odd.} \end{cases} &(2.6) \end{aligned}$$

Therefore

$$x^m = \sum_{n=0}^{m} \binom{m}{n} (m-n-1)!! H_n(x) \tag{2.7}$$

where the sum runs over terms where $m-n$ is even. To enforce this, the summation index is relabeled $m-n=2k$ and by the well-known property of the double factorial, this sum simplifies to Equation (2.4). □

Theorem 2.3 (Three term Hermite recurrence relation). *The Hermite polynomials obey the following three term recurrence relation*

$$H_{n+1}(x) = xH_n(x) - nH_{n-1}(x). \tag{2.8}$$

Proof. Take $f(x) = xH_n(x)$. The formula for the m^{th} term of the Hermite expansion

$$\begin{aligned} d_m &= \frac{1}{m!} \int_{-\infty}^{\infty} \left[x \frac{\partial^m}{\partial x^m} H_n(x) + \binom{m}{1} \frac{\partial^{m-1}}{\partial x^{m-1}} H_n(x) \right] \omega(x) dx &(2.9)\\ &= \binom{n}{m} \int_{-\infty}^{\infty} xH_{n-m}(x) \omega(x) dx + \binom{n}{m-1} \int_{-\infty}^{\infty} H_{n-m+1}(x) \omega(x) dx. &(2.10) \end{aligned}$$

The first integral will only produce a non-zero result when $m = n - 1$, since x is equal to $H_1(x)$, and the second term is only non-zero when $m = n + 1$. Therefore

$$d_m = n\delta_{m,n-1} + \delta_{m,n+1} \tag{2.11}$$

and the three term recurrence relation in Equation (2.8) is obtained. □

Theorem 2.4 (Hermite multiplication Theorem)**.** *The Hermite expansion of $H_n(\gamma x)$ is given by*

$$H_n(\gamma x) = n! \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{1}{2^k k!(n-2k)!} \gamma^{n-2k} \left(\gamma^2 - 1\right)^k H_{n-2k}(x) \tag{2.12}$$

Two lemmas are required for this proof.

Lemma 2.5. *The n^{th} order Hermite polynomial is written in terms of the usual polynomials (the inverse of the "inversion" formula* (2.4)*) by the expression*

$$H_n(x) = n! \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} \frac{(-1)^k}{2^k k!(n-2k)!} x^{n-2k}. \tag{2.13}$$

Proof. Performing a Taylor series of the n^{th} order Hermite polynomial results in the expression

$$H_n(x) = \sum_{m=0}^{n} \binom{n}{m} H_{n-m}(0) x^m. \tag{2.14}$$

The Hermite polynomials evaluated at $x = 0$ are known as the Hermite numbers and only take values for $(n - m)$ even, in which case

$$H_{n-m}(0) = (-1)^{\frac{n-m}{2}} (n - m - 1)!!. \tag{2.15}$$

Therefore relabeling $(n - m) = 2k$ leads to (2.13) again by the well-known expression for the double factorial. □

Lemma 2.6. *The integral of the stretched Hermite polynomial*

$$I_\alpha = \int_{-\infty}^{\infty} H_\alpha(\gamma x)\omega(x)dx \tag{2.16}$$

is only non-zero for even α and has the value

$$I_\alpha = (\alpha - 1)!! \left(\gamma^2 - 1\right)^{\frac{\alpha}{2}}. \tag{2.17}$$

Proof. Lemma 2.5 is used to Taylor expand the Hermite polynomial

$$I_\alpha = \sum_{\beta=0}^{\alpha} \binom{\alpha}{\beta} H_{\alpha-\beta}(0)\gamma^\beta \int_{-\infty}^{\infty} x^\beta \omega(x)dx. \tag{2.18}$$

The Hermite polynomial evaluated at zero is given in Equation (2.15), and is only non-zero when $\alpha - \beta$ is even, and enforce this by writing $\alpha - \beta = 2j$

$$I_\alpha = \sum_{j=0}^{\lfloor \frac{\alpha}{2} \rfloor} \binom{\alpha}{\alpha - 2j} H_{2j}(0)\gamma^{\alpha-2j} \int_{-\infty}^{\infty} x^{\alpha-2j}\omega(x)dx, \tag{2.19}$$

this shows that α must be even as well, as the integral over the polynomial in x is also only non-zero when the exponent is even – this is equivalent to saying the original integral is only non-zero for even α which is true as any odd function will integrate to zero. This is enforced by setting $\alpha = 2M$

$$I_{2M} = \sum_{k=0}^{M} \binom{2M}{2M-2k} (2k-1)!!(2M-2k-1)!! \left(\gamma^2\right)^{M-k} (-1)^k \tag{2.20}$$

which, after using the definition of the double factorial, and the binomial theorem, reduces to

$$I_{2M} = (2M-1)!! \left(\gamma^2 - 1\right)^M . \tag{2.21}$$

□

Hermite multiplication Theorem. Take $f(x) = H_n(\gamma x)$, the m^{th} coefficient in the Hermite expansion is given by

$$d_m = \frac{\gamma^m}{(n-m)!} \int_{-\infty}^{\infty} H_{n-m}(\gamma x)\omega(x)dx. \tag{2.22}$$

This integral is precisely what is calculated in Lemma 2.6. Using this result for the coefficient in Equation (2.22) leads to the simple form

$$d_m = \binom{n}{m} (n-m-1)!!\gamma^m \left(\gamma^2 - 1\right)^{\frac{n-m}{2}} \tag{2.23}$$

whenever $n - m$ is even and equal to zero otherwise, resulting in

$$H_n(\gamma x) = \sum_{m=0}^{n} \binom{n}{m} (n-m-1)!!\gamma^m \left(\gamma^2 - 1\right)^{\frac{n-m}{2}} \tag{2.24}$$

where the sum only runs over even values of m. Making the change of index $n-m = 2k$ recovers Equation (2.12) as needed. □

Theorem 2.7. *The weighted integral of a Hermite polynomial evaluated at the sum $x + y$ has a simple form given by*

$$\int_{-\infty}^{\infty} H_n(x+y)\omega(x)dx = y^n. \tag{2.25}$$

Proof. The n^{th} order Hermite polynomial evaluated at the sum $x + y$ can be Taylor expanded in y to obtain

$$H_n(x+y) = \sum_{m=0}^{n} \binom{n}{m} y^m H_{n-m}(x). \tag{2.26}$$

Reversing the summation variable $k = n - m$ results in a Hermite expansion for $H_n(x+y)$ and therefore the weighted integrals of the derivatives are these coefficients

$$\int_{-\infty}^{\infty} \frac{\partial^k}{\partial x^k} H_n(x+y)\omega(x) = \frac{n!}{(n-k)!} y^{n-k}, \tag{2.27}$$

the $k = 0$ term is precisely Equation (2.25). □

Theorem 1.1 can also be used to provide an alternative proof of the Hermite polynomial linearization theorem [8].

Theorem 2.8 (Hermite Polynomial Linearization Theorem)**.** *The product of two Hermite polynomials can be written as a sum of Hermite polynomials in the following way*

$$H_n(x)H_m(x) = \sum_{j=0}^{\min(n,m)} \binom{m}{j} \binom{n}{j} j! H_{n+m-2j}(x). \tag{2.28}$$

Proof. Set

$$f(x) = H_n(x)H_m(x) = \sum_{\alpha=0}^{n+m} d_\alpha H_\alpha(x). \tag{2.29}$$

The α derivative is given by

$$\frac{\partial^\alpha f(x)}{\partial x^\alpha} = \sum_{\beta=0}^{\alpha} \binom{\alpha}{\beta} \frac{n!}{(n-\beta)!} \frac{m!}{(m-\alpha+\beta)!} H_{n-\beta}(x)H_{m-\alpha+\beta}(x). \tag{2.30}$$

The maximum α can be is $n+m$, which will obtain for at least one term. It is understood at this stage that terms with negative Hermite coefficient are zero, since they arise from the derivative operator acting on $H_0(x)$. The limits of the summation will become more precise below.

When integrating against the Gaussian weighting function, the only term that will be non-zero is when

$$\beta^* = \frac{n-m+\alpha}{2}, \tag{2.31}$$

and this will not occur for every set of $\{n, m, \alpha, \beta\}$. For instance, for β^* to be an integer, α must have the same parity as $n-m$ (or equivalently $n+m$), guaranteeing that the Hermite expansion respects the odd or even nature of the product $H_n(x)H_m(x)$. The expression resulting from the β^* term is

$$\int_{-\infty}^{\infty} \frac{\partial^\alpha f(x)}{\partial x^\alpha} \omega(x)dx = \alpha! \binom{n}{\frac{n+m-\alpha}{2}} \binom{m}{\frac{n+m-\alpha}{2}} \left(\frac{n+m-\alpha}{2}\right)! \tag{2.32}$$

Furthermore, the index on Hermite polynomials can never go below zero, and together with (2.31) gives rise to a lower bound on $\alpha = \max(n-m, m-n)$.

Therefore the Hermite expansion becomes

$$H_n(x)H_n(x) = \sum_{\alpha=\max(n-m,m-x)}^{n+m} \binom{n}{\frac{n+m-\alpha}{2}} \binom{m}{\frac{n+m-\alpha}{2}} \left(\frac{n+m-\alpha}{2}\right)! H_\alpha(x). \tag{2.33}$$

Making the index substitution $j = \frac{n+m-\alpha}{2}$ leads to Equation (2.28). □

2.2 Hermite Expansions

Theorem 1.1 can be used to determine the Hermite expansions of other function of interest, such as the Gaussian distribution function itself.

Theorem 2.9. *The Hermite expansion of the probability distribution function for $\mathcal{N}(0, \sigma^2)$*

$$\omega_\sigma(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{x^2}{2\sigma^2}} \tag{2.34}$$

is

$$\omega_\sigma(x) = \sum_{m=0}^{\infty} \frac{(-1)^m}{m!2^m \sqrt{2\pi\left(\sigma^2+1\right)^{2m+1}}} H_{2m}(x). \tag{2.35}$$

Proof. Successive derivatives of the distribution in Equation (2.34) gives rise to the scaled Hermite polynomials

$$H_n\left(\frac{x}{\sigma}\right) = \frac{(-\sigma)^n}{\omega_\sigma(x)} \frac{\partial^n}{\partial x^n} \omega_\sigma(x) \tag{2.36}$$

and therefore the n^{th} term in the Hermite expansion is given by

$$d_n = \frac{1}{(-\sigma)^n n! \sqrt{2\pi\sigma^2}} \int_{-\infty}^{\infty} H_n\left(\frac{x}{\sigma}\right) \omega_\sigma(x)\omega(x)dx. \tag{2.37}$$

The product $\omega_\sigma(x)\omega(x)$ can be transformed into $\omega(y)$ by the change of variables $y = \frac{x}{\sigma}\sqrt{\sigma^2+1}$. Leading to an integral that is covered by Lemma 2.6

$$d_n = \begin{cases} \frac{1}{\sigma^n n! \sqrt{2\pi(\sigma^2+1)}}(n-1)!! \left(\frac{-\sigma^2}{\sigma^2+1}\right)^{\frac{n}{2}} & n \text{ even} \\ 0 & n \text{ odd.} \end{cases} \tag{2.38}$$

Using the definition of the double factorial and changing the summation to $m = 2n$ results in Equation (2.35). □

Theorem 2.10. *The cumulative distribution function of a normal* $\mathcal{N}(0, \sigma^2)$

$$\Phi_\sigma(x) = \int_{-\infty}^{x} \omega_\sigma(x)dx = \frac{1}{2}\left[1 + \mathit{erf}\left(\frac{x}{\sqrt{2}\sigma}\right)\right] \tag{2.39}$$

has Hermite expansion

$$\Phi_\sigma(x) = \frac{1}{2} + \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)k!2^k\sqrt{2\pi(\sigma^2+1)^{2k+1}}} H_{2k+1}(x) \tag{2.40}$$

Proof. Applying Theorem 1.3 to the function $\omega_\sigma(x)$ results in the series

$$\Phi_\sigma(x) = \int_{-\infty}^{\infty}\int_{-\infty}^{x} \omega_\sigma(y)dy\omega(x)dx + \sum_{n=1}^{\infty} \frac{1}{n} d_{n-1} H_n(x) \tag{2.41}$$

where the d_n are the coefficients of the Hermite expansion of $\omega_\sigma(x)$. Performing the integral and inserting the coefficients leads to

$$\Phi_\sigma(x) = \frac{1}{2} + \sum_{n=1}^{\infty} \begin{cases} \frac{(-1)^{\frac{n-1}{2}}}{n(\frac{n-1}{2})!2^{\frac{n-1}{2}}\sqrt{2\pi(\sigma^2+1)^n}} H_n(x) & n-1 \text{ even} \\ 0 & n-1 \text{ odd} \end{cases}. \tag{2.42}$$

Making the index substitution $2k = n - 1$ leads to Equation (2.40). □

Theorem 2.11. *The Hermite expansion of the indicator function*

$$\mathbb{1}(x) = \begin{cases} 1 & x > 0 \\ \frac{1}{2} & x = 0 \\ 0 & x < 0 \end{cases} \tag{2.43}$$

is

$$\mathbb{1}(x) = \frac{1}{2} + \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k+1)k!2^k\sqrt{2\pi}} H_{2k+1}(x). \tag{2.44}$$

Proof. The indicator function can be written as a limit of the cumulative normal distribution

$$\mathbb{1}(x) = \lim_{\sigma \to 0} \Phi_\sigma(x). \tag{2.45}$$

This limit can be taken on each term in the Hermite expression for $\Phi_\sigma(x)$ resulting in the Hermite expansion for the indicator function given in Equation (2.44). □

3 Gauss-Hermite Quadrature and the Weighted Integral of Derivatives

N^{th} order Gauss- Hermite quadrature (GHQ) approximates Gaussian integrals by a sum

$$I[f] = \int_{-\infty}^{\infty} f(x)\omega(x)dx \approx \sum_{i=0}^{N-1} w_i f(x_i), \tag{3.1}$$

where the weighting function is given in Equation (0.2). The weights abscissa x_i are chosen to be the roots of the N^{th} Hermite polynomial $x_i \in \{x|H_N(x) = 0\}$ of which there are exactly $N-1$ and they are all real (see, for example, Theorem 3.6.12 in Stoer and Bulirsch [11]).

The weights w_i come from the solution of the $N-1$ "tower equations"

$$\sum_{i=0}^{N-1} w_i H_j(x_i) = c_0 \delta_{j0} \tag{3.2}$$

where

$$c_m = \int_{-\infty}^{\infty} H_m^2(x)\omega(x)dx = m! \tag{3.3}$$

The tower equations actually hold for $j \in [0, 2N-1]$ as shown in Theorem 3.6.24 of [11], which states that the error in this approximation

$$E[f] \equiv I[f] - \sum_{i=0}^{N-1} w_i f(x_i) \tag{3.4}$$

is given by

$$E[f] = \frac{f^{(2N)}(\xi)}{(2N)!} c_N \tag{3.5}$$

where ξ is some point in the interval $(-\infty, \infty)$. Therefore any polynomial of degree less than $2N$ will have a vanishing error term, and therefore is exact.

This can be understood intuitively by the following argument: if $f(x)$ is a polynomial of order $2N$, it can be written as $f(x) = H_N(x)q(x) + r(x)$, where the quotient and remainder polynomials, $q(x)$ and $r(x)$ respectively, are of order at most $N-1$. The quotient term vanishes in the Gaussian quadrature technique since the abscissa are chosen to be roots of $H_N(x)$ and the remainder term is exactly integrated by virtue of the tower equations.

It turns out that more than just the integral can be approximated by a single call to GHQ. The same weights and abscissa can be used to approximate the weighted integral of the first M derivatives of the integrand

$$I\left[\frac{\partial^n f}{\partial x^n}\right] = \int_{-\infty}^{\infty} \frac{\partial^n f}{\partial x^n}\omega(x)dx. \tag{3.6}$$

Furthermore, these integrals are precisely $n!$ times the coefficients d_n of the Hermite expansion

$$f(x) = \sum_{n=0}^{\infty} d_n H_n(x), \tag{3.7}$$

which leads to an efficient algorithm to numerically determine these coefficients.

Lemma 3.1. *The error term for Gauss-Hermite quadrature*

$$E[f] = \frac{N!}{(2N)!} f^{(2N)}(\xi') \tag{3.8}$$

bounded by

$$l\frac{N!}{(2N)!} \leq E[f] \leq u\frac{N!}{(2N)!} \tag{3.9}$$

where

$$l = \inf\{f^{(2N)}(x) | x \in [-x_{N-1}, x_{N-1}]\}, \tag{3.10}$$

$$u = \sup\{f^{(2N)}(x) | x \in [-x_{N-1}, x_{N-1}]\} \tag{3.11}$$

and x_{N-1} is the largest zero of $H_N(x)$.

Proof. Theorem 2.1.5.9 in [11] states that for every $\overline{x} \in (-\infty, \infty)$ there exists a point ξ within an interval of the support abscissae such that the error of the interpolating polynomial is

$$f(\overline{x}) - h(\overline{x}) = \frac{H_N^2(\overline{x}) f^{(2N)}(\xi)}{(2N)!}. \tag{3.12}$$

This ξ is therefore bounded by the maximum and minimum support abscissae, which in the case of Gauss-Hermite quadrature, are the zeros of the N^{th} Hermite polynomial. The error (3.12) is integrated against the Gaussian weighting function results in the error of the integral

$$E[f] = \frac{1}{(2N)!}\int_{-\infty}^{\infty} f^{(2N)}(\xi(x)) H_N(x)^2 \omega(x) dx. \tag{3.13}$$

The next step involves the mean value theorem of integral calculus, which results in the derivative term being evaluated at an unknown point $\xi'(x)$ where $x \in (-\infty, \infty)$. However, since ξ' is bounded by the maximal root of $H_N(x)$, a maximum and minimum error can be determined by finding the infimum and supremum of the function inside this range, resulting in the bounds presented in Equation (3.9). □

Theorem 3.2. *Given the weights w_i and abscissa x_i of N^{th} order Gauss-Hermite quadrature, which satisfy*

$$\sum_{i=0}^{N-1} w_i H_j(x_i) = \delta_{j,0} \tag{3.14}$$

$$x_i \in \{x_i | H_N(x_i) = 0\}, \tag{3.15}$$

and an integrand $f(x) \in \mathcal{C}^{(2n)}$ which obeys then the integral of the n^{th} order derivative of $f(x)$, where $n < N$, can be approximated by

$$I\left[\frac{\partial^n f}{\partial x^n}\right] \approx \sum_{i=0}^{N-1} w_i H_n(x_i) f(x_i). \tag{3.16}$$

The leading term in the error of the n^{th} derivative is given by

$$E\left[\frac{\partial^n f}{\partial x^n}\right] = \frac{N!}{(2N-n)!} f^{(2N-n)}(\xi') \tag{3.17}$$

for some $\xi' \in [-x_{N-1}, x_{N-1}]$, where x_{N-1} is the largest root of $H_N(x)$.

Proof. The integral for the n^{th} derivative

$$I\left[\frac{\partial^n f}{\partial x^n}\right] = \int_{-\infty}^{\infty} \frac{\partial^n f(x)}{\partial x^n} \omega(x) dx \tag{3.18}$$

can be integrated by parts n times, at each point we use the property of the integrand in Equation (1.2) to ensure the boundary term vanishes, to obtain

$$I\left[\frac{\partial^n f}{\partial x^n}\right] = \int_{-\infty}^{\infty} f(x)(-1)^n \frac{\partial^n}{\partial x^n} \omega(x) dx. \tag{3.19}$$

This derivative is exactly $\omega(x)H_n(x)$ by the definition of Hermite polynomials in Equation (0.1). Therefore, the integral of the n^{th} derivative is given by the expression

$$I\left[\frac{\partial^n f}{\partial x^n}\right] = \int_{-\infty}^{\infty} f(x)H_n(x)\omega(x)dx, \tag{3.20}$$

which can be approximated by N^{th} order Gauss-Hermite quadrature

$$I\left[\frac{\partial^n f}{\partial x^n}\right] \approx \sum_{i=0}^{N-1} w_i H_n(x_i) f(x_i), \tag{3.21}$$

which is Equation (3.16) as desired.

The error term for the integral of the n^{th} derivative can be found by applying the same method that leads to Equation (3.5) with a new function $g(x) = f(x)H_n(x)$, since $E\left[\frac{\partial^n f}{\partial x^n}\right] = E[f \cdot H_n] = E[g]$. Applying Theorem 3.6.24 in [11] gives the error

$$E[g] = \frac{N!}{(2N)!} g^{(2N)}(\xi') \tag{3.22}$$

for some $\xi' \in [-x_{N-1}, x_{N-1}]$ by Lemma 3.1. Application of the product rule gives

$$g^{(2N)}(x) = \sum_{k=1}^{2N} \binom{2N}{k} \frac{\partial^k}{\partial x^k} H_n(x) f^{(2N-k)}(x) \tag{3.23}$$

which, since $\frac{\partial}{\partial x} H_n(x) = nH_{n-1}(x)$ gives for the error

$$E\left[\frac{\partial^n f}{\partial x^n}\right] = \sum_{k=1}^{n} \binom{n}{k} \frac{N!}{(2N-k)!} H_{n-k}(\xi') f^{(2N-k)}(\xi'). \tag{3.24}$$

Setting $k = n$ produces the term with the lowest derivative of $f(x)$, and gives the leading term shown in Equation (3.17). □

3.1 Error Analysis

To demonstrate the lower and upper bounds numerically, Gauss-Hermite quadrature is used on the simple integrand $f(x) = e^x$. In this case the weighted integral of all order of derivatives is equal to $e^{\frac{1}{2}}$, $l = e^{-x_{N-1}}$ and $u = e^{x_{N-1}}$. The error is still given by Equation (3.17) with $n = 0$, and the error indeed falls between these bounds for all orders of quadrature as shown in Figure 1.

The coefficient $N!/(2N-n)!$ determines the approximation of the weighted integral of the derivative, and increases with n, implying higher order derivatives are less accurate. Furthermore, this coefficient approaches 1 for $n = N$ and therefore the approximation will not be accurate after some order M. In order to determine this level, Stirling's approximation is used ([10]) on Equation (3.17) leading to

$$E\left[\frac{\partial^n f}{\partial x^n}\right] = \frac{1}{e^{N-n}} \frac{N^{N+\frac{1}{2}}}{(2N-n)^{2N-n+\frac{1}{2}}} f^{(2N-n)}(\xi'). \tag{3.25}$$

This approximation is very good for even moderate values of N. For the purposes of this paper, "accurate" will indicate an error that is less than machine precision, $E \approx 10^{-16}$. Therefore, assuming that the derivative term is of order 1, M can be found by solving the following equation

$$N \ln N + N - M - (2N - M) \ln(2N - M) \approx -16 \ln 10 \tag{3.26}$$

for fixed N. The result of solving this transcendental equation numerically are found in Table 1. These points can be seen graphically in Figure 2 as the points where the error in the weighted integral of the n^{th} derivative crosses the horizontal line indicating machine precision.

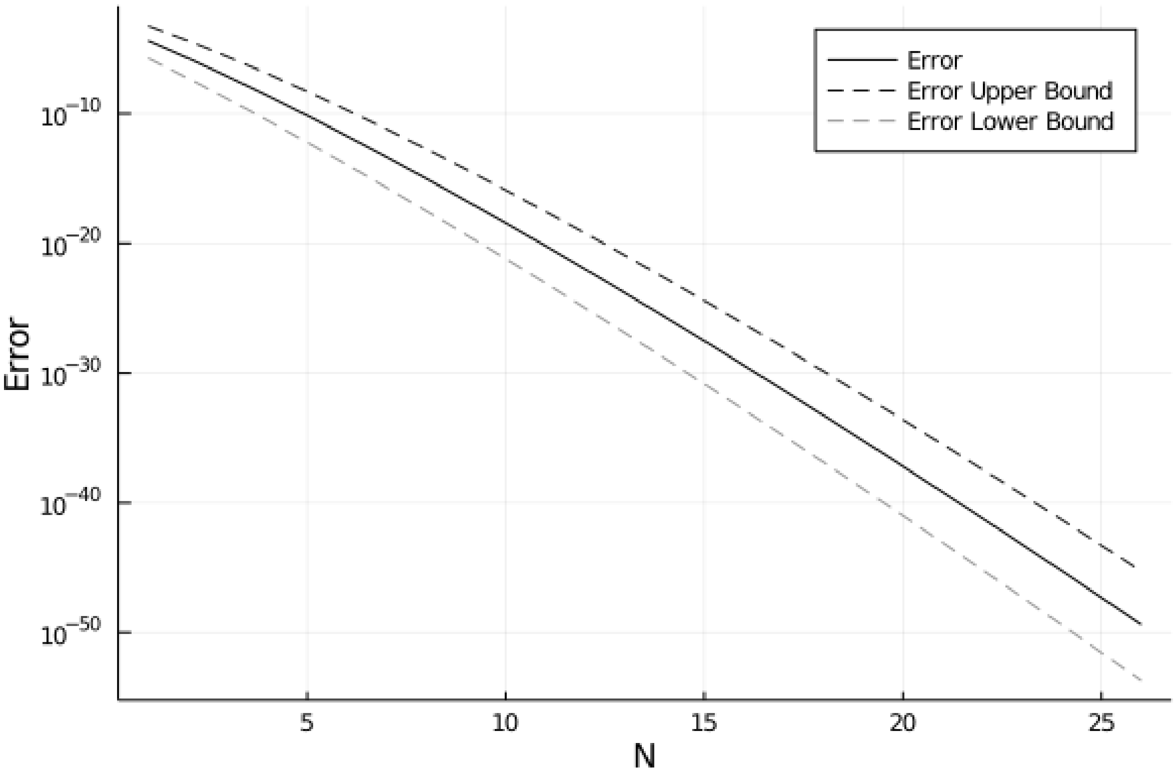

Figure 1: The error of Gauss-Hermite quadrature for the integrand $f(x) = e^x$, together with the lower and upper bounds as defined in the body of the paper, as a function of the order of quadrature.

N	M
10	0
20	9
30	20
40	30
50	41
60	51

Table 1: Order of derivative where the Gauss-Hermite quadrature no longer produces an accurate weighted integral of the derivative.

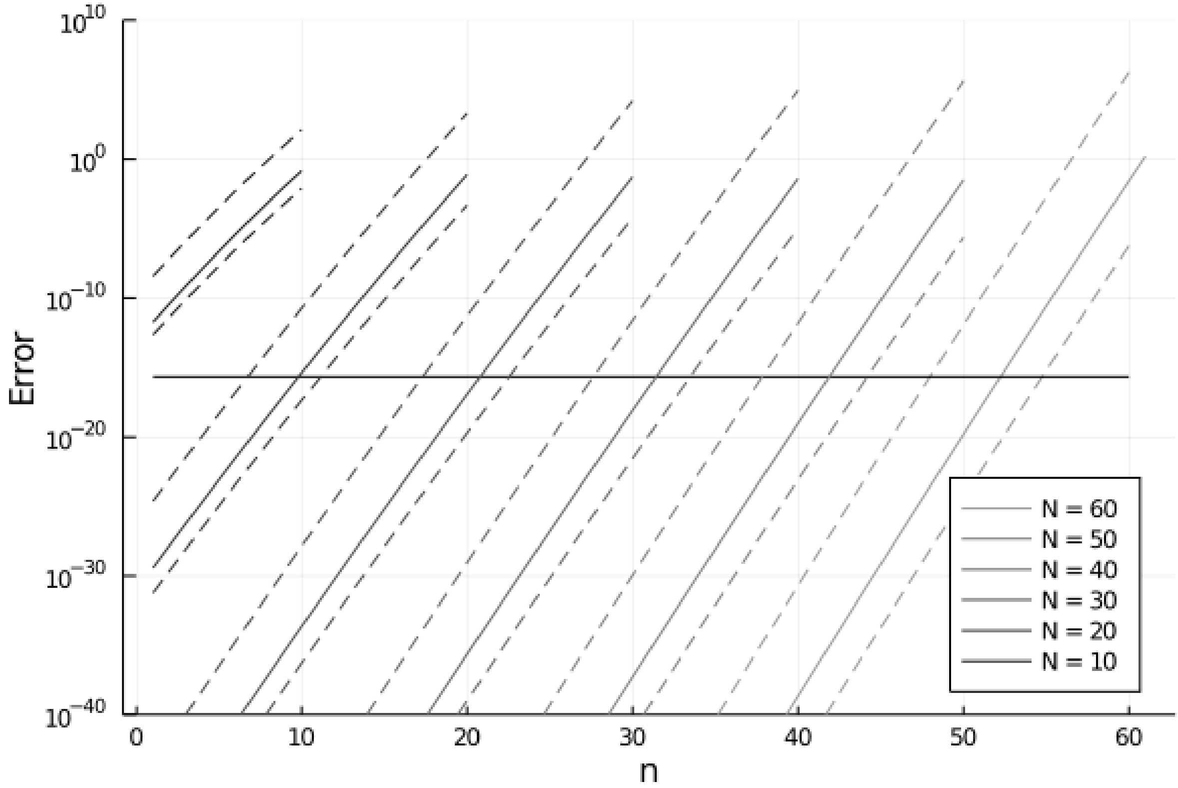

Figure 2: Error in the weighted integral of the n^{th} derivative given by a single call to Gauss-Hermite quadrature, shown orders $N \in [10, 20, 30, 40, 50, 60]$. The horizontal line indicates machine precision $\approx 10^{-16}$, where the routine no longer will provide an accurate result.

3.2 Numerical Hermite Expansion

Theorem 3.2 also lends itself to an algorithm to numerically approximate functions by Hermite polynomials by using a single call to a quadrature method. Naively, one could determine the coefficients in the Hermite expansion via Equation (1.5) for $n \in \{0, M\}$ by calling a quadrature routine $M+1$ times. The following algorithm uses only one single call to a quadrature routine.

Algorithm 1.

Calculate the abscissa $\mathbf{X} = (x_0, x_1, \ldots, x_M)^T$*, and weights* $\mathbf{W} = (w_0, w_1, \ldots, w_{N-1})$ *(one efficient method is the Golub-Welsch algorithm ([5]))*

Calculate the square matrix $\mathcal{H}_{ij} = w_i H_j(x_i), i, j \in [0, N-1]$

Calculate the vector of function evaluations $\mathbf{F} = (f(x_0), f(x_1), \ldots, f(x_{N-1}))$

Form the matrix product $\mathbf{J} = \mathcal{H}\mathbf{F}$

Choose some integer M *where the approximation error is significant*

The Hermite expansion of $f(x)$ *is given by the sum*

$$f(x) \approx \sum_{n=0}^{M} \frac{J_n}{n!} H_i(x) \tag{3.27}$$

As an example, this algorithm is used to numerically determine the Hermite polynomial expansion of the two functions which were of interest calculated in this paper – the normal probability distribution and the normal cumulative distribution function – with the results shows in Figure 3.

4 Conclusion and Remarks

In this paper, a general expression for the coefficients of a Hermite expansion of a function, the integral of a function and the derivative of a function, are derived. These expressions can be used to simply prove many Hermite identities, including a novel proof of the Hermite linearization theorem.

Furthermore, this expressions makes Hermite expansions simple to calculate. As a demonstration, the Hermite expansion of the normal probability distribution function, the cumulative distribution function and the indicator function are presented.

Finally, an efficient algorithm to numerically calculate these coefficients is presented, which is based on Gauss-Hermite quadrature. The paper concludes with an analysis on the error and accuracy of the algorithm.

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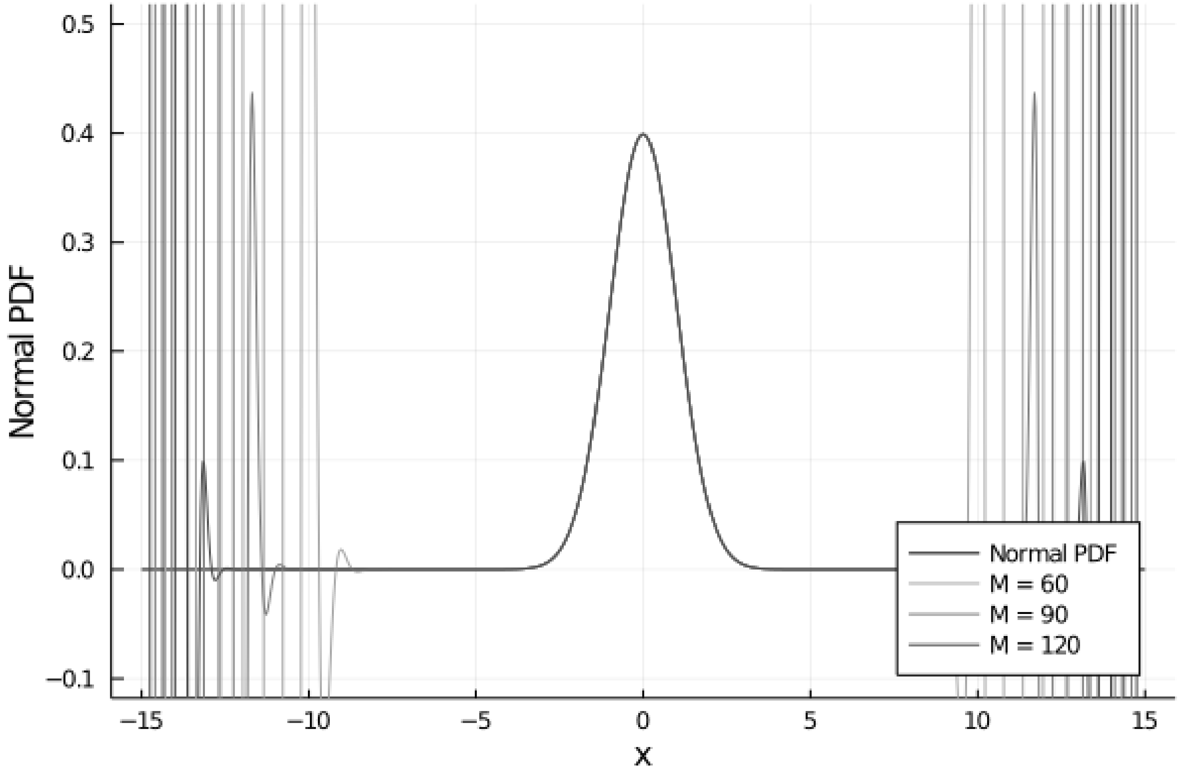

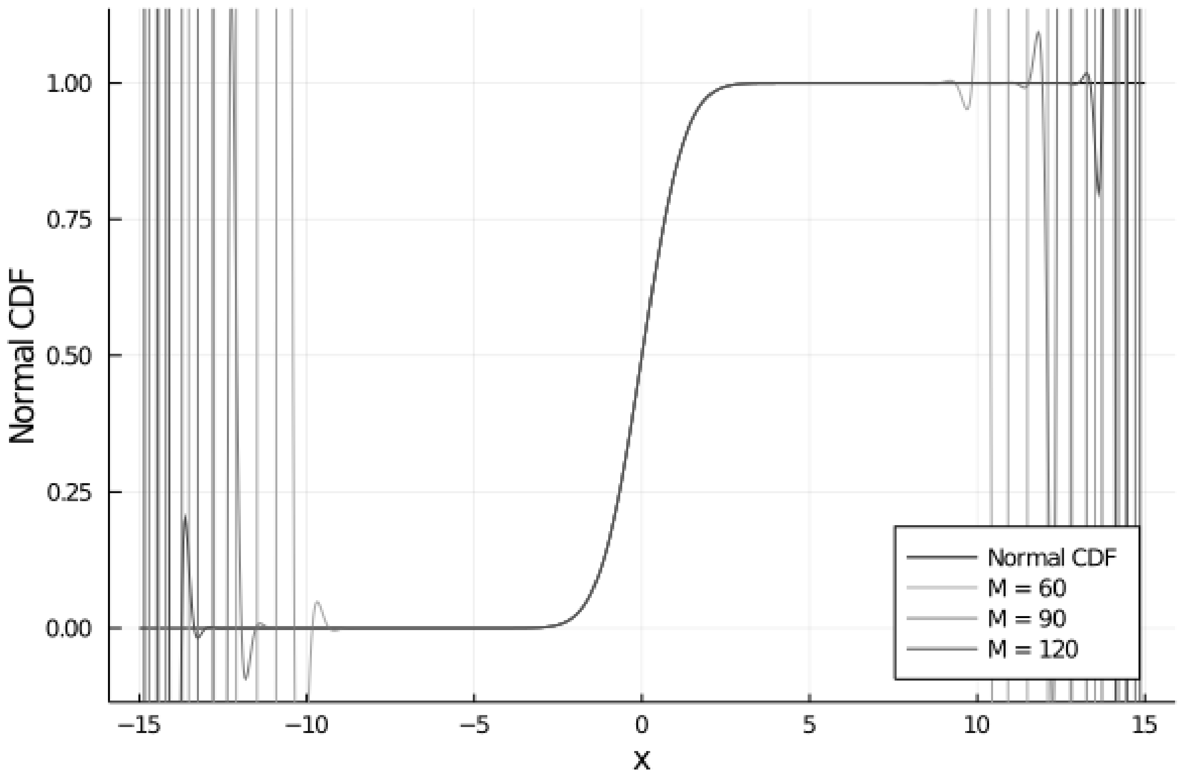

Figure 3: The numerical Hermite expansion of the normal probability function (top) and normal cumulative distribution function (bottom) truncated at orders $60, 90$ and 120 computed by Algorithm 1.

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