Appendix I: Hermite Polynomials

Consider the linear, second-order ordinary differential equation:

$$y'' - 2xy' + 2ny = 0 \quad \text{(A-1)}$$

where n is a non-negative integer and y' and y'' represent the first and second derivatives, respectively, of y with respect to x. By searching for series solutions for y as a function of x, one finds a solution for each n that is a polynomial of order n.[1] For example, if $n = 1$, we see by inspection that $y = 2x$ solves equation (1). Of course, $y = 2x$ is a polynomial of order 1. More generally, let's call the solution for each non-negative integer n $y = H_n(x)$. We've already seen that $H_1(x) = 2x$. We list the first few Hermite polynomials below:

$$H_0(x) = 1$$

$$H_1(x) = 2x$$

$$H_2(x) = 4x^2 - 2$$

$$H_3(x) = 8x^3 - 12x$$

$$H_4(x) = 16x^4 - 48x^2 + 12 \quad \text{(A-2)} .$$

The reader may notice that all the polynomials here would remain solutions of (A-1) after multiplication by any constant. The list we provide is the common convention for choosing the constants to satisfy recurrence relations that facilitate analysis. The leading term of $H_n(x)$ will always be $2^n x^n$.

In (A-2) we listed just the first five Hermite polynomials. Think of the infinite sequence of Hermite polynomials as we let n go from zero to infinity. The functions have the critically important properties that they are orthogonal and complete on the infinite interval $(-\infty, +\infty)$ with the weight function $\exp(-x^2)$. This orthogonality means that

$$\int_{-\infty}^{+\infty} e^{-x^2} \, H_m(x) H_n(x) \, dx = 0 \, , \; m \neq n \quad \text{(A-3)} .$$

As a sketch of the proof of orthogonality, we would re-write (A-1) as

$$\left(e^{-x^2} \, y'\right)' + 2n \, e^{-x^2} \, y = 0 \quad \text{(A-4)}$$

[1] Equation (1) has two linearly independent solutions. We are interested only in the solution that we can represent as a <u>finite</u> series. The solution that we ignore remains an infinite series.

and then evaluate the integral

$$\int_{-\infty}^{+\infty} \left(e^{-x^2}\, y_n'\right)'\, y_m\, dx$$

twice by parts as we show in successive equalities below:

$$\int_{-\infty}^{+\infty} \left(e^{-x^2}\, y_n'\right)'\, y_m\, dx \;=-\int_{-\infty}^{+\infty} y_n' \left(e^{-x^2}\, y_m'\right) dx \;=\; +\int_{-\infty}^{+\infty} \left(e^{-x^2}\, y_m'\right)'\, y_n\, dx \;\; .$$

With these integration-by-parts results and equation (A-4), we find that

$$(n-m) \int_{-\infty}^{+\infty} e^{-x^2}\, y_n\, y_m\, dx \;=\; 0$$

which proves (A-3).

The completeness of the $H_n(x)$ means that any well-behaved function[2] $f(x)$ can be expressed as a linear combination of the $H_n(x)$. That is, there exist coefficients C_n such that

$$f(x) = \sum_{n=0}^{\infty} C_n\, H_n(x) \;\; . \quad \text{(A-5)}$$

We've now exhausted what we need to know about Hermite polynomials. But let's ponder equation (A-5) before we leave. This equation gives us an exact representation of $f(x)$ as an infinite series of Hermite polynomials. We will use this representation later but will find that we can't use all the (infinite number of) terms. Rather, we may use only the first five or ten or twenty. These <u>finite</u> series will be approximations of $f(x)$.

[2] In this discussion, "well behaved" means that $f(x)$ is continuous everywhere except at isolated points where it is permitted to have jump discontinuities.

Appendix II: Gauss Quadrature

Forget Hermite polynomials for a few minutes. The word "quadrature" is a synonym for "numerical integration". If we need to know the integral from zero to four of $f(x)=x^2$, we simply apply the anti-derivative $x^3/3$ and evaluate this entity at the two endpoints to give $64/3$. But if we need to integrate the more difficult function $f(x)=\exp\left(1/_{x+1}\right)$, we must estimate the result numerically. Please remark the word "estimate". All numerical integrations are approximations. The goal of numerical integration is to achieve a desired accuracy with a good estimate of this accuracy for the least amount of computation.

Possibly the simplest form of numerical integration is to look at the mid-point of the interval ($x=2$ in this example where we integrate over the interval $x\in(0,4)$) and approximate the integral as four (the length of the interval) times $f(2)$ (the function evaluated at the mid-point). (This result is 16 and is not a good approximation for $64/3$.) The next simplest method is the Trapezoidal Rule which evaluates the function $f(x)$ at the two endpoints (rather than at just the mid-point). (This Trapezoidal Rule result is 32 and is also a bad approximation.) With computer programs it is elementary to divide any given interval (such as $x\in(0,4)$) into many smaller intervals and apply a method such as the Trapezoidal Rule on the smaller intervals to get better accuracy.

I've got to say, though, that writing a program to apply the Trapezoidal Rule to ever smaller intervals is highly inelegant. It's crude and barbaric. You'll have many brilliant minds of the past three hundreds years spinning in their graves. Before computers, research and discovery of improved numerical integration methods was highly important. Hence, there are many known techniques superior to the Trapezoidal Rule and we will jump to the method that may be the most brilliant.

Gauss Quadrature begins with the specification of an infinite, complete, orthogonal sequence of polynomials in which the domain of the polynomials matches the desired integration interval and the orthogonality condition is consistent with the desired integrand. We choose the Hermite polynomials since they suit our financial risk applications well in terms of both the integration interval and desired integrand. (As the reader may have guessed, Gauss Quadrature with Hermite polynomials is "Gauss-Hermite Quadrature".) More specifically, we will want to approximate integrals of the form

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx$$

in which the e^{-x^2} term denotes either the normal or log-normal probability density functions.

Let's call this integral *I* and use equations (A-5) and (A-3) of this memorandum:

$$I = \int_{-\infty}^{+\infty} e^{-x^2} f(x) dx$$

$$= \int_{-\infty}^{+\infty} e^{-x^2} \sum_{n=0}^{\infty} C_n H_n(x) dx$$

$$= \sum_{n=0}^{\infty} C_n \int_{-\infty}^{+\infty} e^{-x^2} H_n(x) dx$$

$$= C_0 \int_{-\infty}^{+\infty} e^{-x^2} dx = \sqrt{\pi}\, C_0 \quad \text{(A-6)} .$$

This is outstanding! The end result is simple. The desired integral I is just the square root of π multiplied by the coefficient of the zero-th order Hermite polynomial. Hence, all we need to do is get the expansion of the function $f(x)$ in terms of the Hermite polynomials and then use just the zero-th order coefficient C_0. If we can accomplish this task, then equation (A-6) is an exact result. In practice, though, we will expand $f(x)$ into a finite series of Hermite polynomials as an approximation. The approximation improves as we increase the number of terms.

With the approximation

$$f(x) \approx \sum_{i=0}^{n} C_i\, H_i(x) \;, \quad (\mathrm{A}-7)$$

we can solve a linear system of equations to get the C_0 to apply in equation (A-6):

$$I = \int_{-\infty}^{+\infty} dx\, e^{-x^2} f(x) = \sqrt{\pi}\; C_0 \;\approx \sum_{i=0}^{n} w_i\, f(x_i) \;\; (\mathrm{A}-8)$$

In (A-8), the x_i are the $n+1$ zeroes of $H_{n+1}(x)$ and the w_i are the coefficients we construct by solving the linear equations that force equation (A-7) to be exactly correct at the points x_i. Fortunately, both the x_i and the w_i are tabulated[3] and we have created a web application to generate these values. We don't need to re-derive them. The sum of the w_i is $\sqrt{\pi}$. In arriving at (A-8) we have omitted a long discussion of why we choose zeroes of $H_{n+1}(x)$ for the x_i and why the approximation in (A-8) is much more accurate than one would imagine.

[3] See, for example, R. E. Greenwood and J. J. Miller, "Zeros of the Hermite Polynomials and Weights for Gauss' Mechanical Quadrature Formula," *University of Texas*, 1948.

Additional Section Excluded from GARP Article to Explain High-Order Accuracy of Gauss-Hermite Quadrature

Let's take an example to make this real. We want to approximate

$$I = \int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx$$

with the first three Hermite polynomials: $H_0(x); H_1(x); H_2(x)$. (See equations (A-2).) To get the "best fit", I will choose three points on the abscissa (*x*-axis) and force the approximation

$$f(x) \approx C_0 H_0(x) + C_1 H_1(x) + C_2 H_2(x) \quad \text{(A-9)}$$

to be exact at these three points (which we'll call $x_0, x_1,$ and x_2). We will choose these three values to be 0, $+\sqrt{3/2}$, and $-\sqrt{3/2}$. These may seem like arbitrary choices, but we'll circle back to this choice in just a minute. For now, note that applying equation (A-9) to each of the points $x_0, x_1,$ and x_2 gives three linear equations in the three unknowns $C_0, C_1,$ and C_2. It's quite easy to solve these equations since the $H_n(x)$ have even or odd symmetry depending on whether *n* is even or odd and our three points $x_0, x_1,$ and x_2 are symmetric about zero. Further, we only need to get C_0. Of course, this C_0 depends on the function value $f(x)$ at all three points $x_0, x_1,$ and x_2. With minimal algebra, we find

$$I = \int_{-\infty}^{+\infty} e^{-x^2} f(x)\,dx = \sqrt{\pi}\, C_0 = \frac{\sqrt{\pi}}{6}\left[f\left(-\sqrt{3/2}\right) + 4 f(0) + f\left(+\sqrt{3/2}\right)\right]$$

Now let's get back to the pressing question of why we choose the $x_0, x_1,$ and x_2 as we did. First, we need three points to find the three unknowns $C_0, C_1,$ and C_2.[4] Second, it is helpful that these points be symmetric about zero. Most fascinating is that these $x_0, x_1,$ and x_2 are the zeroes of the *next* Hermite polynomial $H_3(x)$. Why would we do that? Why does $H_3(x)$ matter? In short, the answer is we get the "right answer" for C_0 by doing the work for the equation (A-9) approximation with the first three Hermite polynomials $H_0(x); H_1(x); H_2(x)$ while, in reality, extending the approximation to $H_3(x)$. Stated differently, once we find C_0 with the approximation of the first three Hermite polynomials, we know immediately that we'd still get the same C_0 if we improve the approximation to four Hermite polynomials. The accuracy of our approximation is better than we expect.

[4] The reader might object that we only care about C_0. But we still count the other two unknowns for purposes of determining how many abscissa values are necessary.

The most immediate method to prove this property is to consider the linear system of equations we solved to get $C_0, C_1, \text{and } C_2$. If we keep the three abscissa points $x_0, x_1, \text{and } x_2$ and then add a third point x_3 in order to compute C_3, the matrix of the linear system has three zeroes (since $H_3(x)$ is zero at the points $x_0, x_1, \text{and } x_2$) that tell us immediately that the prior $C_0, C_1, \text{and } C_2$ values are correct and we have just one remaining equation for C_3 in terms of the $C_0, C_1, \text{and } C_2$. (Below we give a different argument that reaches this same conclusion.)

But the story gets even stranger. We just found that an approximation to order *n* is actually correct to order $n+1$ (due to our choice of the zeroes of $H_{n+1}(x)$ for the abscissa points in the order *n* approximation). It's even better than this. We find the correct integral (*i.e.*, C_0) for integrand functions $f(x)$ all the way to order *2n*!

I could not recall the proof of this amazing property nor did I find it in the references I consulted. Yet it forms a key justification for applying Gauss Quadrature methods. So I managed to derive the proof and find it to be both obscure and brilliant. That's a bad combination! Brilliant observations are usually simple in their final form. There's likely a more elegant proof than what I'll describe here.

In determining the weights w_i, we inadvertently forced the equality

$$\sum_{i=-k}^{+k} w_i \, H_j(x_i) = 0, \quad j = 1, \cdots, 2k \quad \text{(A-10)}$$

where we assume our approximation is to order *2k*. (As a simplification of sorts, we now let the index *i* have symmetric negative and positive values.) To verify this non-obvious claim, let's develop the solution C_0 for the special (and simple) case $k = 1$. Equation (A-9) in matrix form is

$$\begin{pmatrix} H_0(x_{-1}) & H_1(x_{-1}) & H_2(x_{-1}) \\ H_0(x_0) & H_1(x_0) & H_2(x_0) \\ H_0(x_{+1}) & H_1(x_{+1}) & H_2(x_{+1}) \end{pmatrix} \begin{pmatrix} C_0 \\ C_1 \\ C_2 \end{pmatrix} = \begin{pmatrix} f(x_{-1}) \\ f(x_0) \\ f(x_{+1}) \end{pmatrix}$$

By Cramer's Rule, we find C_0 as the ratio of two matrix determinants Δ_n / Δ_d. The denominator determinant, Δ_d, is that of the left-hand side "Hermite matrix:"

$$\Delta_d = \begin{vmatrix} H_0(x_{-1}) & H_1(x_{-1}) & H_2(x_{-1}) \\ H_0(x_{-1}) & H_1(x_0) & H_2(x_0) \\ H_0(x_{+1}) & H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix} .$$

The numerator determinant, Δ_n, is

$$\Delta_n = \begin{vmatrix} f(x_{-1}) & H_1(x_{-1}) & H_2(x_{-1}) \\ f(x_0) & H_1(x_0) & H_2(x_0) \\ f(x_{+1}) & H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix} \ . \quad \text{(A-11a)}$$

We can write out Δ_n by Laplace Expansion with the co-factors as elements of the left column as

$$\Delta_n = f(x_{-1}) \begin{vmatrix} H_1(x_0) & H_2(x_0) \\ H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix} - f(x_0) \begin{vmatrix} H_1(x_{-1}) & H_2(x_{-1}) \\ H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix}$$

$$+ f(x_{+1}) \begin{vmatrix} H_1(x_{-1}) & H_2(x_{-1}) \\ H_1(x_0) & H_2(x_0) \end{vmatrix} \quad \text{(A-11b)}$$

Here’s the point that matters – the *2x2* matrix determinants of (A-11b) are proportional to the weights w_i that multiply the $f(x_i)$ as in equation (A-8). Thus, (A-11a) and (A-11b) allow us to prove (A-10) by substituting the column

$$\begin{matrix} H_j(x_{-1}) \\ H_j(x_0) \\ H_j(x_{+1}) \end{matrix} \ \text{ for } \ \begin{matrix} f(x_{-1}) \\ f(x_0) \\ f(x_{+1}) \end{matrix} \ \text{ with } j = 1,2$$

in equation (A-11a). Making this substitution, we create

$$\begin{vmatrix} H_j(x_{-1}) & H_1(x_{-1}) & H_2(x_{-1}) \\ H_j(x_0) & H_1(x_0) & H_2(x_0) \\ H_j(x_{+1}) & H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix} = 0 \ , \ j = 1,2 \quad \text{(A-11c)}$$

This expression in (A-11c) is zero for *j=1,2* since the matrix is singular (repeated columns) and the determinant of a singular matrix is zero. Hence we prove (A-10) and this proof is valid for arbitrary values of *k* with *j* ranging from 1 to 2*k*.

Equation (A-11c) is equivalent to (A-10) for the case of $k = 1$. Now consider setting $j = 3$ in (A-11c). The equation remains satisfied (*i.e.*, the determinant has zero value) because the Gauss method deliberately chooses the zeroes x_{-1}, x_0, x_{+1} such that $H_3(x) = 0$ at each x_{-1}, x_0, x_{+1}. What that means is that the actual function $f(x)$ may have (and likely does have) a non-zero component proportional to $H_3(x)$. But that component does not alter the value of C_0 expressed as

$$C_0 = \frac{\Delta_n}{\Delta_d} = \begin{vmatrix} f(x_{-1}) & H_1(x_{-1}) & H_2(x_{-1}) \\ f(x_0) & H_1(x_0) & H_2(x_0) \\ f(x_{+1}) & H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix} \Big/ \Delta_d$$

since the $f(x)$ values at x_{-1}, x_0, x_{+1} are unchanged by the $H_3(x)$ component.

Finally, for this $k = 1$ case, let’s imagine that $f(x)$ has a component $H_4(x)$ - which it likely does. Modifying (A-11c) again, it is *also* true that

$$\begin{vmatrix} H_4(x_{-1}) & H_1(x_{-1}) & H_2(x_{-1}) \\ H_4(x_0) & H_1(x_0) & H_2(x_0) \\ H_4(x_{+1}) & H_1(x_{+1}) & H_2(x_{+1}) \end{vmatrix} = 0$$

To prove this point, we note a tremendously valuable recurrence relation for Hermite polynomials:

$$H_{j+1}(x) = 2xH_j(x) - 2jH_{j-1}(x) \quad \text{(A-12)}$$

Choosing $j = 3$ to get an expression for $H_4(x)$,

$$H_4(x) = 2xH_3(x) - 6H_2(x)$$

The determinant above with $H_4(x)$ in the left column will have zero value since we know already that the components $2xH_3(x)$ and $6H_2(x)$ each produce zero value for the determinant.

Recapping this $k = 1$ example, then, we expressed $f(x)$ as an expansion to order $2k$ (=2) (see equation (A-9)). We chose the three abscissa points to fit this Hermite polynomial expansion, labeled as x_{-1}, x_0, x_{+1}, to be the zeroes of $H_3(x)$. We then showed that the C_0 we discover in this polynomial fitting does not change even if $f(x)$ actually does have components of $H_3(x)$ and $H_4(x)$. Since it is the C_0 that determines the integral approximation, our approximation is valid to order 4 even though we employed polynomials only to order 2. Hence, we double the order of the integral evaluation with the Gauss technique.

To show that this doubling of the order of the integral approximation is valid for larger values of k, we need one additional concept. We begin again with equation (A-10) which we reprise below:

$$\sum_{i=-k}^{+k} w_i \; H_j(x_i) = 0\,, \qquad j = 1, \cdots, 2k$$

Our earlier explanation for this identity still stands. The numerator determinant in the expression for C_0, after substituting $H_j(x_i)$ for $f(x_i)$ in the left-most column with j taking values from 1 to $2k$, vanishes since the implied matrix is singular. Also as before, (A-10) is valid for $j = 2k + 1$ since we choose the x_i as zeroes of $H_{2k+1}(x)$ and (A-10) is valid for $j = 2k + 2$ when we apply the recurrence relation (A-12).

To continue extending the validity of (A-10) to yet higher values of j, we need to prove and use:

$$\sum_{i=-k}^{+k} w_i \; x_i \; H_j(x_i) = 0; \quad j = 2, \cdots, 2k+1 \quad (\text{A}-13\text{a})$$

$$\sum_{i=-k}^{+k} w_i \; x_i^2 \; H_j(x_i) = 0; \quad j = 3, \cdots, 2k+1 \quad (\text{A}-13\text{b})$$

$$\text{generally,} \sum_{i=-k}^{+k} w_i \; x_i^m \; H_j(x_i) = 0; \;\; j = m+1, \cdots, 2k+1; \;\; m = 0, \cdots, 2k \;\; (\text{A}-13\text{c})$$

We prove (A-13a) by first re-arranging (A-12) as

$$2xH_j(x) = H_{j+1}(x) + 2jH_{j-1}(x) \;\; \text{all } j > 0 \quad \text{(A-14)}$$

Then, multiplying by w_i, evaluating at x_i, and summing over *i*,

$$\sum_{i=-k}^{+k} 2w_i x_i H_j(x_i) = \sum_{i=-k}^{+k} w_i H_{j+1}(x_i) + \sum_{i=-k}^{+k} 2jw_i H_{j-1}(x_i) \quad (\text{A}-15\text{a})$$

Both summations on the right-hand side of (A-15a) are zero when *j* takes values 2 to 2*k*+1. Thus, we've reproduced (A-13a). Proving (A-13b) requires just another step: multiply (A-14) by xw_i, evaluate at x_i, and sum over *i* to get

$$\sum_{i=-k}^{+k} 2w_i x_i^2 H_j(x_i) = \sum_{i=-k}^{+k} w_i x_i H_{j+1}(x_i) + \sum_{i=-k}^{+k} 2jw_i x_i H_{j-1}(x_i) \quad (\text{A}-15\text{b})$$

By reference to (A-15a), we see immediately that both summations on the right-hand side of (A-15b) are zero when *j* takes values 3 to 2*k*. Hence, the left-hand side of (A-15b) vanishes for these same *j* values. But we know also that the left-hand summation is zero for $j = 2k + 1$. Thus, we've reproduced (A-13b).

A fascinating twist is that the validity of (A-15b) for $j = 2k + 1$ implies that the first summation on the right-hand side of this (A-15b) is zero. That tells us that the preceding (A-15a) is valid for $j = 2k + 2$. *This* deduction moves us to recognize that the first summation on the right-hand side of (A-15a) is zero which then extends the validity of (A-10) to $j = 2k + 3$. Each step in our proof of (A-13a) to (A-13b) to the general (A-13c) extends the range of *j* values that satisfy (A-10). The extension ends because the lower limit of *j* in (A-13a) to (A-13b) to (A-13c) creeps higher to eliminate the identity after 2*k* steps. It is this step-by-step extension from the initial order of the approximation 2*k* by another 2*k* steps that provides the "double accuracy" of Gauss quadrature. A key element of our algebraic manipulations is the identity $H_{2k+1}(x_i) = 0$ arising from our choice of the x_i as the zeroes of $H_{2k+1}(x)$.

Let's generalize and conclude. In equation (A-9) we posited an approximation to a function $f(x)$ to order 2 (*i.e.*, to $H_2(x)$). Extending this approximation to order 2*k* we write

$$f(x) \approx \sum_{j=0}^{2k} C_j \, H_j(x) \quad (\mathrm{A}-16)$$

We then derive the integral approximation

$$I = \int_{-\infty}^{+\infty} e^{-x^2} f(x) \, dx = \sqrt{\pi} \, C_0 = \sum_{i=-k}^{+k} w_i \, f(x_i) \quad (\mathrm{A}-17)$$

in which the x_i are the $2k+1$ zeroes of $H_{2k+1}(x)$ and the w_i are the coefficients we construct by solving the linear equations that force equation (A-16) to be exactly correct at the points x_i. Fortunately, both the x_i and the w_i are tabulated[5] and we have created a web application to generate these values. We don't need to re-derive them. The sum of the w_i is $\sqrt{\pi}$.

[5] See, for example, R. E. Greenwood and J. J. Miller, "Zeros of the Hermite Polynomials and Weights for Gauss' Mechanical Quadrature Formula," *University of Texas*, 1948.