Distributed Approximating Functionals

Theory and Computational Methodology

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Abstract

The abstract goes here after the paper is done.

I. INTRODUCTION

The distributed approximating functionals (DAF) method was developed and implemented for solving classes of differential equations very accurately with a high fidelity to the accuracy of derivatives. The DAF method was applied first to time-dependent propgation problems in theoretical quantum physics applications[? ? ? ? ? ? ?].

The DAF method has been used in various situations that involve time evolution, from quantum particle trajectories[?], integration of Feynman path integrals[?], and fluid dynamics[? ?], and also as a method of solving bound eigenvalue-eigenvector problems[? ?] and data interpolation[?].

The DAF method is more computationally intensive in practice than other simpler methods, however, much can be precomputed and reused, so the most time consuming aspects of the method need be computed only once

1. **Differential Equations**: The DAF method constructs matrix operators that can be applied to multidimentional linear differential equations.

2. **Interpolation**: The DAF method can be used to approximate functions and their derivatives with high accuracy.

II. MATHEMATICAL BACKGOUND

In this section, we develop the mathematical foundation for the DAF method, establish the needed relations to employ the DAF in practice, and define its limitations.

A. Hermite Expansion of Delta Functions

The DAF method uses an approximation of the Dirac delta function generated by an expansion in Hermite polynomials. With the appropriate Gaussian weight function, the Hermite polynomials form a complete and orthogonal basis on the domain of $(-\infty, \infty)$. This basis set can be used to expand any function on this domain. The advantages of this method include high degrees of accuracy in representing other functions, and provides an analytic, functional approximation of undefined functions such as what might be represented by discrete data points.

The expansion follows the general formula[**?**] of

$$\delta(x) = \sum_{m=0}^{\infty} h_m H_m\left(\frac{x}{\sigma}\right) e^{-\left(\frac{x}{\sigma}\right)} \tag{1}$$

Where H_m are the Hermite polynomials, σ is a scaling function, and h_m are the expansion coefficients. A few notes on these terms:

- $H_m(x)$: There are two common definitions for the Hermite polynomials, which are referred to commonly as the *probability* and the *physics* definitions, which here we follow Wikipedia's notation and use H_m for the physics definition and He_m for the probabilistic. They are related by $He_m = 2^m H_m$. In this document, we use the physics definition.

- σ: The scaling function σ can be used to scale the Hermite functions "horizontally". In the practical case in which the infinite sum in equation 1 is limited to a finite number of terms, the σ factor directly effects how many terms are needed to represent a function. A poorly chosen value of σ can make converging the summation very difficult.

- h_m: The expansion coefficients represent how much each Hermite term contributes to the expansion. These can be derived analytically for the $\delta(x)$ expansion. This derivation is shown below.

To determine the expansion coefficients h_m, we begin with equation 1 and multiply each side by $H_n(x/\sigma)$ and integrate over $(-\infty, \infty)$,

$$\int_{-\infty}^{\infty} H_n\left(\frac{x}{\sigma}\right) \delta(x) dx = \int_{-\infty}^{\infty} H_n\left(\frac{x}{\sigma}\right) \sum_{m=0}^{\infty} h_m H_m\left(\frac{x}{\sigma}\right) e^{-\left(\frac{x}{\sigma}\right)} dx \tag{2}$$

$$H_n(0) = \sum_{m=0}^{\infty} h_m \int_{-\infty}^{\infty} H_n\left(\frac{x}{\sigma}\right) H_m\left(\frac{x}{\sigma}\right) e^{-\left(\frac{x}{\sigma}\right)} dx \tag{3}$$

Next we use the orthogonality property[**? ?**] of

$$\int_{-\infty}^{\infty} H_m(x) H_n(x) e^{-x^2} dx = \sqrt{\pi}\, 2^m m!\, \delta_{mn} \tag{4}$$

where δ_{mn} is the Kronecker Delta function and is equal to 1 if $m = n$ and 0 otherwise. With a scaling factor, σ, this becomes

$$\int_{-\infty}^{\infty} H_m\left(\frac{x}{\sigma}\right) H_n\left(\frac{x}{\sigma}\right) e^{-\left(\frac{x}{\sigma}\right)^2} dx = \sigma\sqrt{\pi}\, 2^m m!\, \delta_{mn} \tag{5}$$

Using this in equation 3, we have

$$H_n(0) = \sum_{m=0}^{\infty} h_m \sigma \sqrt{\pi}\, 2^m m!\, \delta_{mn}$$

which gives

$$h_n = \frac{H_n(0)}{\sigma\sqrt{\pi}\, 2^n\, n!} \tag{6}$$

One thing that can be observed by this definition is that for all odd values of n, the coefficient h_n is zero because $H_n(0) = 0$ for all odd-order Hermite polynomials. This makes sense when we consider that the Dirac delta function is symmetric in x, and therefore only even Hermite functions, i.e. those that are also symmetric in x, will contribute to the expansion series.

Note that we can use the Hermite polynomial recurrsion relation, given as

$$H_{n+1}(x) = 2xH_n(x) - 2nH_{n-1}(x) \tag{7}$$

to quickly find the coefficients. We can see that the first several h_n are

$$\begin{aligned} h_0 &= 1 \\ h_1 &= 0 \\ h_2 &= 2 * 0 * H_1(0) - 2 * 1 * H_0(0) = -2 \\ h_3 &= 0 \\ h_4 &= 2 * 0 * H_3(0) - 2 * 3 * -2 = 12 \\ &\ldots \end{aligned}$$

From this we define a function, $\Delta_{\sigma,M}(x)$ that depends parametrically on σ and M, and is exact as $M \to \infty$,

$$\Delta_{\sigma,M}(x) = \sum_{m=0}^{M} h_m H_m\left(\frac{x}{\sigma}\right) e^{-\left(\frac{x}{\sigma}\right)^2} \tag{8}$$

III. APPLICATION

Here we assess some test cases to show how the DAF method functions in practice. and with this function, we can approximate any function with

$$f(x) = \int f(y)\Delta_{\sigma,M}(y-x)\mathrm{d}y \tag{9}$$

Note here also that taking the derivative with respect to x in the above equation gives

$$\frac{\mathrm{d}}{\mathrm{d}x} f(x) = \int f(y) \frac{\mathrm{d}}{\mathrm{d}x} \left[\Delta_{\sigma,M}(y-x) \right] \mathrm{d}y \tag{10}$$

where we note that on the right side, the derivative applies only to the Δ term. Since this is an expansion of polynomials and weight functions, the derivative is analytic.

A. One-Dimensional

In a one-dimensional DAF application, we consider a continuous domain in x from which we have have discrete set of abscissas where we have samples of the function $f(x)$.

The function $f(x)$ is known only at the set of discrete points $[x_n]$. There are many methods to fit these data points to an analytic function so that it is easier to work with. The DAF method has some advantages that make it very appealing for some cases.

Let's assume we have a set of coordinate points, $(x_0, f_0), (x_1, f_1), ...$ that represent some measured data or a given function. The set of x values we will describe as $\mathbf{x}$ and we have

$$f(\mathbf{x}) = \mathbf{f}$$

where $\mathbf{x}, \mathbf{f}$ are sets of discrete points, and any of these individual points will be referenced as x_i, for example.

Next we define another set of points along the x axis. These are the points at which we want values or derivatives for the function $f(x)$. This we call $\bar{\mathbf{x}}$ **Note** that x and $\bar{x}$ are coordinates on the same x-axis, but represent different, independent coordinates. This is important, because formally we are using the DAF method as an operator to transform discrete points $\mathbf{x}$ into an analytic funtion on the domain of $\bar{\mathbf{x}}$. This can be tricky to keep straight, but it is important because some times we will operate $\mathbf{x}$ space and sometimes on $\bar{\mathbf{x}}$.

From the properties of the $\delta(x)$ function, we can now write an identity for calculating a single point of f in the domain of x (not $\bar{x}$).

$$f(\bar{x}_i) = \int \delta(\bar{x}_i - x) f(x) \mathrm{d}x \tag{11}$$

Now, we only know the values of f at the points x, so in practice this integral will be a summation of some form with appropriate weight factors, w_i.

$$f(\bar{x}_i) = \sum_j w_j \delta(\bar{x}_i - x_j) f(x_j) \tag{12}$$

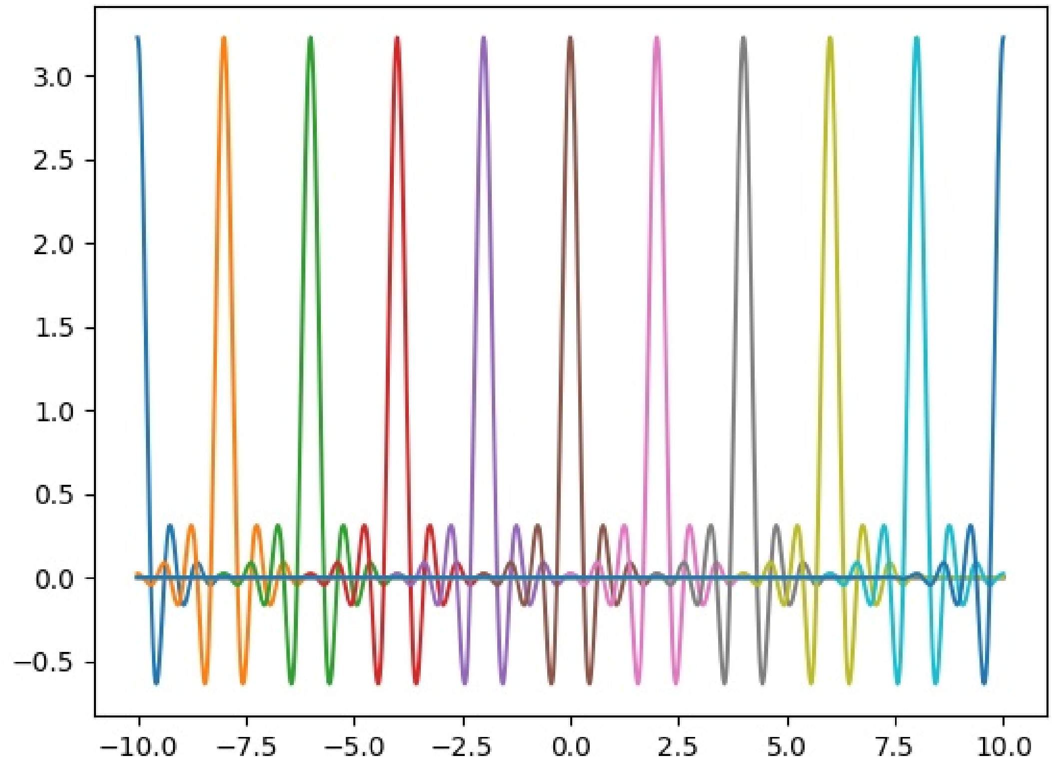

FIG. 1: Delta functions at a given set of x points.

Next, we replace the δ function with the expansion defined in equation 8 to get the following...

$$f(\bar{x}_i) = \sum_j w_j \delta(\bar{x}_i - x_j) f(x_j) \tag{13}$$

$$f(\bar{x}_i) = \sum_j w_j \Delta_{\sigma,M}\left(\frac{x_i - \bar{x}_j}{\sigma}\right) f(x_j) \tag{14}$$

$$f_i = \sum_j \mathbf{D}_{\sigma M,ij}\mathbf{f}_j \tag{15}$$

Where we have defined $\mathbf{D}_{\sigma M,ij}$ as the combination of the integration weights, w_j and the δ function expansion. Note that σ and M are parameters that are used to tune the DAF method for better accuracy, and the indices i, j indicate the points in x and $\bar{x}$ space. For simplicity, from here on we drop the σ and M specifiers from the notation, and define

$$\mathbf{D}_{ij} = w_j \Delta_{\sigma,M}(x_i - \bar{x}_j) = w_j \sum_{m=0}^{M} h_m H_m \left(\frac{x_i - \bar{x}_j}{\sigma} \right) e^{-\left(\frac{x_i - \bar{x}_j}{\sigma}\right)^2} \tag{16}$$

and we define $\mathbf{D}_{ij}$ to be the *DAF Operator* in one dimension.

With the DAF operator defined by given parameters of σ and M, we can see that it is indexed by two labels, one for x space and one for $\bar{x}$ space. Since we included the integration weights into the definition, we can now write

$$f_j = \sum_i \mathbf{D}_{ij} f_i \tag{17}$$

which is equivalent to a vector-vector multiply,

$$f_j = (D_{0j}, D_{1j}, D_{2,j}, ...) \begin{pmatrix} f_0 \\ f_1 \\ f_2 \\ ... \end{pmatrix} \tag{18}$$

B. Multi-Dimensional

In a multi-dimensional application, we use the DAF to approximate a function such as

$$f(\bar{x}, \bar{y}, \bar{z}) = \iiint f(x, y, z) \delta(\bar{x} - x) \delta(\bar{y} - y) \delta(\bar{z} - z) \mathrm{d}x \mathrm{d}y \mathrm{d}z \tag{19}$$

or in vector notation for simplicity:

$$f(\bar{\mathbf{r}}) = \int_{\mathbf{V}} f(\mathbf{r}) \delta(\bar{\mathbf{r}} - \mathbf{r}) \mathrm{d}\mathbf{r} \tag{20}$$

where $\delta(\mathbf{r}) = \delta(r_1)\delta(r_2)\delta(r_3)...$ and $\mathbf{V}$ is the multi-dimensional volume to which the DAF is being applied.

In three spacial dimensions, these coordinates are typically x, y, and z, but the method is not limited to strictly spacial coordinates, nor is it limited to the number of dimensions.

IV. ITEMS TO INCLUDE IN TEXT

NOTE: Toeplitz Matrices?

NOTE: The points at which values or derivatives of the function are wanted must be known before construction of the DAF matrices.

NOTE: Specialized DAF cases: periodic, symmetric. In multidimensional DAF applications, it might be good to label them by the irreducible representation.

Appendix A: Proof of Lobatto Integration Formula

1. General Quadrature Proof

A Gaussian-type quadrature formula for approximating an integral is based off of a set of polynomials that are orthogonal with respect to a weighting function over the range of integration. For the Legendre polynomials, the range of integration is $[-1, 1]$ and the weight function is 1.

For any given set of n quadrature abscissas,$\{x\}_n$, weights can be calculated to make the following summation exact,

$$\int_{-1}^{1} f(x)\mathrm{d}x = \sum_{i=1}^{n} w_i f(x_i) \tag{A1}$$

for all f if f is a polynomial of order $n-1$ or less. An improvement can be made by specifying a set of abscissas. In the example of Legendre polynomials (and this holds true for other orthogonal polynomials and their related quadrature formulas), the set of points is chosen to be the roots of the $P_n(x)$ Legendre polynomial. Using these abscissas and then calculating the weights ensures a quadrature that will exactly integrate any polynomial of order $2n-1$. This can be shown as follows [**?**],

Say $g(x)$ is a polynomial of order no greater than $2n-1$. This polynomial can be written as

$$g(x) = q(x)P_n(x) + r(x) \tag{A2}$$

where $q(x)$ is the dividend after dividing $g(x)$ by $P_n(x)$, and $r(x)$ is the remainder. If $g(x)$ is of order $2n-1$ or less, then both $q(x)$ and $r(x)$ cannot be of order greater than $n-1$. As such, both $q(x)$ and $r(x)$ can be represented as a linear combination of the set of Legendre polynomials of order $n-1$ and less. Integrating equation A2 gives,

$$\int_{-1}^{1} g(x)\mathrm{d}x = \int_{-1}^{1} q(x)P_n(x)\mathrm{d}x + \int_{-1}^{1} r(x)\mathrm{d}x \tag{A3}$$

$$\int_{-1}^{1} g(x)\mathrm{d}x = 0 + \int_{-1}^{1} r(x)\mathrm{d}x \tag{A4}$$

where the first term on the right-hand side is necessarily zero because if $q(x)$ can be represented by an expansion in Legendre polynomials of orders less then n, then each of these polynomials are orthogonal to $P_n(x)$ with respect to integration. Therefore, all that is left is the integration over the remainder term. In performing the same steps by quadrature,

$$\sum_{i=1}^{n} g(x_i)w_i = \sum_{i=1}^{n} q(x_i)P_n(x_i)w_i + \sum_{i=1}^{n} r(x_i)w_i \tag{A5}$$

$$\sum_{i=1}^{n} g(x_i)w_i = 0 + \sum_{i=1}^{n} r(x_i)w_i \tag{A6}$$

where again the first summation on the right-hand side is zero because the abscissa points were chosen to be the roots of $P_n(x)$. Because $r(x)$ is of order $n-1$ or less, this term can be integrated exactly by quadrature, and thus $g(x)$ is integrated exactly. Thus for any polynomial $g(x)$ of order $2n-1$, the n point quadrature can be made to be exact, giving

$$\int_{-1}^{1} g(x)\mathrm{d}x = \sum_{i=1}^{n} g(x_i)w_i \tag{A7}$$

2. Lobatto Quadrature Proof

The Lobatto integration formula is

$$\int_{-1}^{1} f(x) \approx \frac{2}{n(n-1)}\left[f(-1)+f(1)\right] + \sum_{i=2}^{n-1} w_i f(x_i) \tag{A8}$$

where the abscissas, x_i are the i^{th} root of $P'_{n-1}(x)$, $P_n(x)$ being the n^{th} Legendre polynomial, and the interior weights, w_i are given by the formula

$$w_i = \frac{2}{n(n-1)[P_{n-1}(x)]^2} \tag{A9}$$

This integration quadrature is exact for all functions $f(x)$ such that $f(x)$ is a polynomial of order $2n-3$ or less. The proof of this relies on the Legendre Polynomial recursion relation [**?**],

$$(n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x) \tag{A10}$$

and the Legendre polynomial derivative formula [**?**]

$$(1-x^2)P'_n(x) = -nxP_n(x) + nP_{n-1}(x) \tag{A11}$$

$$= (n+1)\left[xP_n(x) - P_{n+1}(x)\right] \tag{A12}$$

The main difference between the Lobatto Quadrature formula and other Gaussian-type quadratures is that the end points of the integration range ($[-1,1]$, generally) are included as quadrature points. By including these points explicitly, two degrees of freedom are lost, and thus the quadrature is not as accurate as the general case.

By including the end points, the abscissas for Lobatto quadrature are the roots of the equation

$$\Phi_n(x) = (1 - x^2)P'_{n-1}(x) \tag{A13}$$

That these abscissas are those that provide the maximum accuracy is proven in a subsequent section.

The function $\Phi_n(x)$ is a polynomial of order n and has roots at $x = -1, 1$. From the relations given in equations A10 and A11, equation A13 can be rewritten,

$$\begin{aligned}\Phi_n(x) &= (1 - x^2)P'_{n-1}(x) \\ &= (n-1)P_{n-2}(x) - (n-1)xP_{n-1}(x) \\ &= (n-1)P_{n-2}(x) - \frac{n-1}{2n-1}\left(nP_n(x) + (n-1)P_{n-2}(x)\right) \\ &= \frac{n(n-1)}{2n-1}\left(P_{n-2}(x) - P_n(x)\right)\end{aligned} \tag{A14}$$

From here the proof proceeds in the same way as in the general case. Given a polynomial, $g(x)$ that is of order $2n-3$ or less, it can be written similarly to equation A2, but now we use the Φ function instead of a Legendre Polynomial as the divisor,

$$\begin{aligned}g(x) &= q(x)\Phi_n(x) + r(x) \\ g(x) &= q(x)\frac{n(n-1)}{2n-1}\left(P_{n-2}(x) - P_n(x)\right) + r(x)\end{aligned} \tag{A15}$$

If $g(x)$ is of order $2n-3$ or less, then $q(x)$ is of order $n-3$ or less. The remainder $r(x)$ is of order $n-1$ or less, as the highest order possible of the remainder is always one less than then divisor. Preceding as before by integrating both sides gives

$$\int_{-1}^{1} g(x)\mathrm{d}x = \int_{-1}^{1} q(x)\frac{n(n-1)}{2n-1}\left(P_{n-2}(x) - P_n(x)\right)\mathrm{d}x + \int_{-1}^{1} r(x)\mathrm{d}x \tag{A16}$$

In general, the first term on the right-hand side is only zero if $q(x)$ can be expanded in Legendre Polynomials of order $n-3$ or less, due to the presence of the $P_{n-2}(x)$ polynomial. It is possible that $q(x)$ have order $n-1$, but only if $q(x)$ and $P_{n-2}(x)$ remain orthogonal, and this is generally not the case. After integration, we again have the condition

$$\int_{-1}^{1} g(x)\mathrm{d}x = \int_{-1}^{1} r(x)\mathrm{d}x \tag{A17}$$

Performing the Lobatto quadrature on equation A15 behaves similarly to the general quadrature case.

$$\sum_{i=1}^{n} g(x_i)w_i = \sum_{i=1}^{n} q(x_i)w_i \frac{n(n-1)}{2n-1}\left(P_{n-2}(x_i) - P_n(x_i)\right) + \sum_{i=1}^{n} r(x_i)w_i$$
$$\sum_{i=1}^{n} g(x_i)w_i = 0 + \sum_{i=1}^{n} r(x_i)w_i \tag{A18}$$

where again the first term on the right-hand side is zero because the quadrature abscissas were chosen to be roots of $\Phi(x)$ (as defined in equation A14).

Therefore it is proved that the n-point Lobatto Quadrature is exact for all polynomials of order $2n-3$.

3. Proof of Weight Formula for Lobatto Quadrature

Because the Lobatto integration formula exactly integrates any polynomial of order $2n-3$ or less, integrating a Lagrange interpolating polynomial can be done by quadrature exactly. A Lagrange interpolating polynomial is defined in equation **??** and rewritten here for convenience,

$$\lambda_k(x) = \prod_{j\neq k}^{n} \frac{(x-x_j)}{(x_k-x_j)}$$

where $\lambda_k(x_k) = 1$ by definition and is zero at all other quadrature abscissas. Integrating this function produces the quadrature result,

$$\int_{-1}^{1} \lambda_k(x)\mathrm{d}x = \sum_{i=1}^{n} \lambda_k(x_i)w_i$$
$$= w_k\lambda_k(x_k) = w_k \tag{A19}$$

Therefore a formula for the integration of $\lambda_k(x)$ will result in an expression for the weight factors.

The Lagrange interpolating polynomial can also be written in another form based on the Legendre Polynomials. Since the $\lambda_k(x)$ functions share all the same roots as the expression $(1-x*2)P'_{n-1}(x)$ except for the k^{th} root, $\lambda_k(x)$ can be defined as

$$\lambda_k(x) = Q\frac{(1-x^2)P'_{n-1}(x)}{(x-x_k)} \tag{A20}$$

where Q is a normalizing factor that ensures $\lambda_k(x_k) = 1$. The normalization factor Q can be calculated by use of l'Hopital's rule applied to $\lambda_k(x)$ or more simply by the identity [?]

$$\lambda_k(x) = \frac{\Phi(x)}{(x - x_k)\Phi'(x_k)} \tag{A21}$$

where $\Phi(x) = (1-x^2)P'_{n-1}(x)$ and is also defined in equations A13 and A14. Equation A21 is easy to prove given that all terms in $\Phi'(x)$ that contain the $(x-x_k)$ factor after differentiation are zero when $\Phi'(x)$ is evaluated at $x = x_k$. The result is that with normalizing,

$$\lambda_k(x) = \frac{(1 - x^2)P'_{n-1}(x)}{(x - x_k)(1 - x_k^2)P''(x_k)} \tag{A22}$$

It is now left to prove that integrating this expression for $\lambda_k(x)$ gives the weight formula defined in equation A9

$$\begin{aligned}
\int_{-1}^{1} \lambda_k(x)\mathrm{d}x &= \int_{-1}^{1} \frac{(1 - x^2)P'_{n-1}(x)}{(x - x_k)(1 - x_k^2)P''_{n-1}(x_k)} \\
&= \frac{1}{(1 - x_k^2)P''_{n-1}(x_k)} \int_{-1}^{1} \frac{(1 - x^2)P'_{n-1}(x)}{(x - x_k)} \\
&= \frac{2}{n(n-1)[P_{n-1}(x_k)]^2} & \text{(A23)} \\
&= \frac{2n}{(1 - x_k^2)P''_{n-1}(x_k)P'_n(x_k)} & \text{(A24)}
\end{aligned}$$

Where the forms for the weights in equations A23 and A24 are given in references [?] and [?] respectively. From equation A24 we can see the proof of the weights reduces to proving the equality

$$\int_{-1}^{1} \frac{(1 - x^2)P'_{n-1}(x)}{(x - x_k)}\mathrm{d}x = \frac{2n}{P'_n(x_k)} \tag{A25}$$

From here we shall prove that the interior abscissas are indeed the roots of $P'_{n-1}(x)$ and show how to perform the integral in equation A25 to get the formulae for the associated weights.

a. Abscissas

As noted before, the interior weights can be calculated from the solution to the integral

$$\int_{-1}^{1} \lambda_i(x)\mathrm{d}x = w_i \tag{A26}$$

where $\lambda_i(x)$ is the Lagrange interpolating polynomial defined by the chosen abscissas. For the Lobatto quadrature, the interior abscissas are defined to be the roots of $P'_{n-1}(x)$, where $P_n(x)$

is the n^{th} Legendre polynomial and n is the total number of quadrature points (including the end points).

This section proves that the best possible abscissas are the roots of $P'_{n-1}(x)$ and proves the formula, equation A9, for the weights.

First let us presume that we do not know the interior abscissas, but that the end point abscissas have been forced. Earlier in equation A13, Φ was defined as the polynomial with roots at all of the abscissas. Now let us redefine this function as one in which the interior abscissas are unknown,

$$\Phi_n(x) = (1-x^2)\phi_{n-2}(x) \tag{A27}$$

where $\phi_{n-2}(x)$ is some unknown function with $n-2$ real, distinct roots in the range of $[-1,1]$. Here we will follow the formulation of Hildebrand [?], chapters 7-8, on quadratures with assigned abscissas. By the methods of section A 1 we know that maximum accuracy of the quadrature is obtained by using the roots of an orthogonal polynomial. We therefore make the assertion that ϕ_{n-2} is the $(n-2)^{th}$ member of a set of orthogonal polynomials that are orthogonal with respect to the weighting function $\bar{w} \equiv (1-x^2)$. Based on this assertion, we must ensure that ϕ_{n-2} is orthogonal to all polynomials of degree $n-3$ or less. For simplicity in notation, from here on we will set $r = n-2$. Thus,

$$\int_{-1}^{1} \bar{w}(x)\phi_r(x)g_{r-1}(x)\mathrm{d}x = 0 \tag{A28}$$

where $g_{r-1}(x)$ is any general polynomial of degree $r-1$ or less. Following section 7.5 of Hildebrand[?], we proceed to reform equation A28 through successive integration-by-parts. In doing so we require the r^{th} integral of $\bar{w}(x)\phi_r(x)$, and so we define this to be the r^{th} derivative of a function $U_r(x)$,

$$\bar{w}(x)\phi_r(x) = \frac{d^r U_r(x)}{dx^r} = U_r^{(r)}(x) \tag{A29}$$

and from this equation A28 is now

$$\int_{-1}^{1} U_r^{(r)}(x)g_{r-1}(x)\mathrm{d}x = 0 \tag{A30}$$

After r derivatives, the $g_{r-1}(x)$ function is zero and the integral term vanishes. What is left is $r-1$ surface terms given as

$$\begin{aligned}\Big\{U_r^{(r-1)}(x)g_{r-1}^{(1)}(x) - U_r^{(r-2)}(x)g_{r-1}^{(2)}(x) + U_r^{(r-3)}(x)g_{r-1}^{(3)}(x) + \ldots \\ \ldots + (-1)^{r-1}U_r(x)g_{r-1}^{(r-1)}(x)\Big\}\Big|_{-1}^{+1} = 0\end{aligned} \tag{A31}$$

That the sum of the surface terms is zero is necessary to ensure that the integral in equation A30 is zero. Because $g_{r-1}(x)$ can be *any* polynomial of degree $r-1$ or less, there are no constraints on its value at $x = \pm 1$. Therefore, we have the constraint on $U_r(x)$ that

$$U_r^{(r-k)}(-1) = U_r^{(r-k)}(1) = 0, \qquad k = 1, 2, \ldots, r \tag{A32}$$

Furthermore, we have the requirement that if $\phi_r(x)$ is a polynomial of degree r, its $(r+1)^{th}$ derivative must vanish. From this requirement and equation A29, $U_r(x)$ must be a solution to the differential equation

$$\frac{d^{r+1}}{dx^{r+1}}\left[\frac{1}{\bar{w}(x)}\frac{d^r U_r(x)}{dx^r}\right] = \frac{d^{r+1}}{dx^{r+1}}\left[\frac{1}{(1-x^2)}\frac{d^r U_r(x)}{dx^r}\right] = 0 \tag{A33}$$

where $U_r(x)$ must satisfy the conditions of equation A32.

From looking at equation A33, we can see that the $1/(1-x^2)$ term may be problematic; no number of successive derivatives cause this term to vanish. Therefore, this term must be cancled from the $U_r^{(r)}(x)$ term. Still requiring that equation A33 be zero then allows $U_r(x)$ to be a polynomial of order $2r+2$. The requirement of equation A31 leads us to try a function for $U_r(x)$ of the form

$$U_r(x) = C_{r,1}\frac{d^2}{dx^2}(x^2-1)^{r+2} - C_{r,2}(x^2-1)^r \tag{A34}$$

Where $C_{r,1}$ and $C_{r,2}$ is a constant coefficient. Clearly this function has an order of $2r+2$, and though it may seem strange to chose this function, the reasons will be made clear shortly. We are free to choose these coefficients provided that the roots of ϕ_r remain the same and the requirement of equation A31 is maintained. The use of the (x^2-1) terms ensure that the conditions of equation A31 are met; each term in the first r derivatives of this definition of $U_r(x)$ contain at least on (x^2-1) term and are thus zero at $x = \pm 1$. After r applications of the derivative operator with respect to x and division by $\bar{w}(x)$, $U_r^{(r)}(x)$ is a polynomial of order $r = n-2$, and thus also satisfies the condition of equation A33, which is to say the $(r+1)^{th}$ derivative of this polynomial is zero. Hence, all conditions on the form of $U_r(x)$ are met.

In order to find $\phi_r(x)$, we must work out the explicit form of $U_r^{(r)}(x)$. We first apply the derivative operators, and since the conditions from the surface terms are met, those of equation A31, by the (x^2-1) terms, we are free to manipulate the coefficients later. Applying d^r/dx^r to equation A34, we have

$$\frac{d^r}{dx^r}U_r(x) = C_{r,1}\frac{d^{r+2}}{dx^{r+2}}(x^2-1)^{r+2} - C_{r,2}\frac{d^r}{dx^r}(x^2-1)^r \tag{A35}$$

Observing that there is a similarity in this terms to the Rodrigues formula for the Legendre polynomials, defined as

$$P_l(x) = \frac{1}{2^l l!}\frac{d^l}{dx^l}(x^2-1)^l \tag{A36}$$

We can simplify this equation by the choice of the coefficients to be

$$C_{r,1} = -C\frac{(r+1)(r+2)}{2r+1}\frac{1}{2^{r+2}(r+2)!} \tag{A37}$$

$$C_{r,2} = C\frac{(r+1)(r+2)}{2r+1}\frac{1}{2^r r!} \tag{A38}$$

and rewrite equation A35 as

$$\frac{d^r}{dx^r}U_r(x) = -C\frac{(r+1)(r+2)}{2r+1}\left[\frac{1}{2^{r+2}(r+2)!}\frac{d^{r+2}}{dx^{r+2}}(x^2-1)^{r+2} - \frac{1}{2^r r!}\frac{d^r}{dx^r}(x^2-1)^r\right] \tag{A39}$$

$$\frac{d^r}{dx^r}U_r(x) = -C\frac{(r+1)(r+2)}{2r+1}\left[P_{r+2}(x) - P_r(x)\right] \tag{A40}$$

again with $r = n-2$, then we have the following algebraic sequence,

$$\frac{d^r}{dx^r}U_r(x) = -\frac{C(r+1)(r+2)}{2r+1}\left[P_{r+2}(x) - P_r(x)\right] \tag{A41}$$

$$\frac{d^{n-2}}{dx^{n-2}}U_{n-2}(x) = -\frac{Cn(n-1)}{2n-1}\left[P_n(x) - P_{n-2}(x)\right] \tag{A42}$$

$$= C\frac{-n^2+n}{2n-1}\left[P_n(x) - P_{n-2}(x)\right] \tag{A43}$$

$$= C\frac{n^2 - n(2n-1)}{2n-1}P_n(x) - \frac{n(n-1)}{2n-1}P_{n-2}(x) \tag{A44}$$

$$= C\frac{n^2}{2n-1}P_n(x) - nP_n(x) - \frac{n(n-1)}{2n-1}P_{n-2}(x) \tag{A45}$$

$$= C\left(nxP_{n-1}(x) - nP_n(x)\right) \tag{A46}$$

$$= C(1-x^2)P'_{n-1}(x) \tag{A47}$$

where the step between lines A45 and A46 utilizes the three-term recurrance relationship of

$$nxP_{n-1}(x) = \frac{n^2}{2n-1}P_n(x) + \frac{n(n-1)}{2n-1}P_{n-2}(x) \tag{A48}$$

and between lines A46 and A47 the Legendre derivative equation is used,

$$(1-x^2)P'_{n-1}(x) = nxP_{n-1}(x) + nP_n(x) \tag{A49}$$

Placing $U_r^{(r)}(x) = C(1-x^2)P'_{r+1}(x) = (1-x^2)P'_{n-1}(x)$ into equation A33 gives

$$\frac{d^{n-1}}{dx^{n-1}}\left[\frac{1}{(1-x^2)}C(1-x^2)P'_{n-1}(x)\right] = 0 \tag{A50}$$

which is true, being that $P'_{n-1}(x)$ is a polynomial of order $n-2$, the $(n-1)^{th}$ derivative of it must vanish. Therefore, the polynomial that we are seeking, $\phi_{n-2}(x)$, is equal or proportional to $P'_{n-1}(x)$. The coefficient C is determined such that the lowest order polynomial of this set, $\phi_0(x) = CP'_1(x) = 1$ which give $C = 1$. Therefore, $\phi_{n-2}(x) = P'_{n-1}(x)$, and is a member of a set that are orthogonal with respect to the weighting function $(1 - x^2)$.

This proves that for an n point quadrature including the end points, the interior abscissas are in fact the roots of $P'_{n-1}(x)$.

b. End Point Weights

Following is the proof for the end-point weights for the Lobatto Quadrature. From equation A8 we can see that at the end points of $x = \pm 1$ the quadrature weight is $2/(n(n-1))$. To prove this we need to evaluate the integral of equation A25 for the abscissas $x = \pm 1$. For $x = 1$, this is

$$\int_{-1}^{1} \frac{\beta(1-x^2)P'_{n-1}(x)}{(1-x)} \mathrm{d}x = w_{x=1} \tag{A51}$$

where β is the normalization factor to ensure that the polynomial is equal to 1 at $x = 1$. Because the numerator factors directly, l'Hopital's rule is unnecessary to find the normalization, and the integral can be written simply as

$$\int_{-1}^{1} \frac{(1+x)P'_{n-1}(x)}{2P'_{n-1}(1)} \mathrm{d}x = w_{x=1} \tag{A52}$$

First we must evaluate the expression $2P'_{n-1}(1)$. The first several values of $P'_m(x = 1)$ are

$$\begin{aligned} P'_0(1) &= 0 \\ P'_1(1) &= 1 \\ P'_2(1) &= 3 \\ P'_3(1) &= 6 \\ P'_4(1) &= 10 \end{aligned} \tag{A53}$$

and so on. From observation we can see there is a formula of

$$P'_n(1) = \sum_{i}^{n} i = \frac{n(n+1)}{2} \tag{A54}$$

This relation can also be proved from the recursion relation and the definition of the Legendre polynomials. Using equation A54 to rewrite equation A52 gives

$$\int_{-1}^{1} \frac{(1+x)P'_{n-1}(x)}{n(n-1))}\mathrm{d}x = w_{x=1} \tag{A55}$$

This integral can now be evaluated by integration-by-parts,

$$\begin{aligned} n(n-1)w_{x=1} &= \int_{-1}^{1} (1+x)P'_{n-1}(x)\mathrm{d}x \\ &= \int_{-1}^{1} P'_{n-1}(x)\mathrm{d}x + \int_{-1}^{1} xP'_{n-1}(x)\mathrm{d}x \\ &= P_{n-1}(x)|_{-1}^{1} + xP_{n-1}(x)|_{-1}^{1} - \int_{-1}^{1} P_{n-1}(x)\mathrm{d}x \\ &= P_{n-1}(1) - P_{n-1}(-1) + P_{n-1}(1) + P_{n-1}(-1) - 0 \\ &= P_{n-1}(1) + P_{n-1}(1) \\ &= 2 \end{aligned} \tag{A56}$$

Note that $P_l(1) = 1$ for all l, and the integral over any Legendre polynomial other than $P_0(x)$ is zero. Since n represents the number of points in the integration, a one point quadrature is meaningless, since at the very least we count the end points. Therefore, we can rule out the integral over P_{n-1} surviving. Thus for $w_{x=1}$ we have

$$w_{x=1} = \frac{2}{n(n-1)} \tag{A57}$$

just as in equation A8.

For the weight at $x = -1$, the procedure is very similar, but because the Legendre polynomials are alternatively even and odd, their values at $x = -1$ alternate between ± 1 and the derivatives, while still the same magnitude as those at $x = 1$, also alternate between positive and negative. The formula for the derivative value at $x = -1$ is

$$P'_{n-1} = \frac{1}{2}(-1)^n n(n-1) \tag{A58}$$

The integral to be solved is

$$\int_{-1}^{1} \frac{(-1)^n(1-x)P'_{n-1}(x)}{n(n-1))}\mathrm{d}x = w_{x=1} \tag{A59}$$

and proceding as before in equation A56

$$\begin{aligned}
n(n-1)w_{x=-1} &= \int_{-1}^{1}(1-x)P'_{n-1}(x)\mathrm{d}x \\
&= \int_{-1}^{1} P'_{n-1}(x)\mathrm{d}x - \int_{-1}^{1} xP'_{n-1}(x)\mathrm{d}x \\
&= P_{n-1}(x)|_{-1}^{1} - xP_{n-1}(x)|_{-1}^{1} + \int_{-1}^{1} P_{n-1}(x)\mathrm{d}x \\
&= P_{n-1}(1) - P_{n-1}(-1) + P_{n-1}(1) + P_{n-1}(-1) - 0 \\
&= P_{n-1}(-1) + P_{n-1}(-1) = 2(-1)^n
\end{aligned} \tag{A60}$$

which gives

$$w_{x=-1} = \frac{(-1)^n 2}{(-1)^n n(n-1)} = \frac{2}{n(n-1)} \tag{A61}$$

and so the values of the weights at $x = \pm 1$ are proved.

c. *Interior Weights*

Here we wish to prove that the values for the interior integration weights is given by the formulae,

$$w_i = \frac{2}{n(n-1)[P_{n-1}(x)]^2} = -\frac{2n}{(1-x_i^2)P''_{n-1}(x_i)P'_n(x_i)} \tag{A62}$$

Beginning with equation A25 and the knowledge that $P'_{n-1}(x)$ is the $(n-2)^{th}$ member of a set of polynomials orthogonal with respect to $(1-x^2)$, we can now exactly calculate the integral,

$$\int_{-1}^{1} \frac{(1-x^2)P'_{n-1}(x)}{(x-x_i)}\mathrm{d}x = \frac{2n}{P'_n(x_i)}$$

where x_i is the i^{th} root of $P'_{n-1}(x)$.

Keeping the simpler notation of $\phi_r(x) = P'_{n-1}(x)$ with $r = n-2$, we make use of the Christoffel-Darboux identity [**?**],

$$\sum_{k=0}^{m} \frac{\phi_k(x)\phi_k(y)}{\gamma_k} = \frac{\phi_{m+1}(x)\phi_m(y) - \phi_m(x)\phi_{m+1}(y)}{a_m\gamma_m(x-y)} \tag{A63}$$

where $a_m = A_{m+1}/A_m$ with A_m is the coeffcient of the x^m term of $\phi_m(x)$, and γ_m is defined as

$$\gamma_m = \int_{-1}^{1} w(x)\left(\phi_m(x)\right)^2 \mathrm{d}x \tag{A64}$$

Now we define $y = x_i$, where x_i is the i^{th} root of the $\phi_m(x)$ polynomial. With this definition, equation A63 becomes,

$$\sum_{k=0}^{m} \frac{\phi_k(x)\phi_k(x_i)}{\gamma_k} = \frac{-\phi_m(x)\phi_{m+1}(x_i)}{a_m\gamma_m(x-x_i)} \tag{A65}$$

Multiplying both sides of equation A65 by $(1-x^2)\phi_0(x)$ and integrating gives

$$\begin{aligned}
\int_{-1}^{1}(1-x^2)\phi_0(x)\sum_{k=0}^{m}\frac{\phi_k(x)\phi_k(x_i)}{\gamma_k}\mathrm{d}x &= \int_{-1}^{1}(1-x^2)\phi_0(x)\frac{-\phi_m(x)\phi_{m+1}(x_i)}{a_m\gamma_m(x-x_i)}\mathrm{d}x \\
\sum_{k=0}^{m}\frac{\phi_k(x_i)}{\gamma_k}\int_{-1}^{1}(1-x^2)\phi_0(x)\phi_k(x)\mathrm{d}x &= \int_{-1}^{1}(1-x^2)\phi_0(x)\frac{-\phi_m(x)\phi_{m+1}(x_i)}{a_m\gamma_m(x-x_i)}\mathrm{d}x \\
\frac{\phi_0(x_i)}{\gamma_0}\gamma_0 &= \int_{-1}^{1}\frac{-(1-x^2)\phi_0(x)\phi_m(x)\phi_{m+1}(x_i)}{a_m\gamma_m(x-x_i)}\mathrm{d}x \\
\phi_0(x_i) = 1 &= \frac{\phi_{m+1}(x_i)}{a_m\gamma_m}\int_{-1}^{1}(1-x^2)\phi_0(x)\frac{-\phi_m(x)}{(x-x_i)}\mathrm{d}x \\
\frac{-a_m\gamma_m}{\phi_{m+1}(x_i)} &= \int_{-1}^{1}(1-x^2)\phi_0(x)\frac{\phi_m(x)}{(x-x_i)}\mathrm{d}x
\end{aligned} \tag{A66}$$

Now changing back to Legendre polynomials, we have

$$\int_{-1}^{1}\frac{(1-x^2)P'_{n-1}(x)}{x-x_i}\mathrm{d}x = \frac{-a_{n-1}\gamma_{n-1}}{P'_n(x_i)} \tag{A67}$$

The leading coefficients of the Legendre polynomials is given by $A_n = (2n)!/[2^n(n!)^2]$, and therefore the leading coefficients of $P'_n(x)$, A'_n, are given by

$$A'_n = \frac{n(2n)!}{2^n(n!)^2} \tag{A68}$$

$$a_{n-1} = \frac{A'_n}{A'_{n-1}} \tag{A69}$$

$$= \frac{n(2n)!2^{n-1}((n-1)!)^2}{(n-1)(2n-2)!2^n(n!)^2} \tag{A70}$$

$$= \frac{2n-1}{n-1} \tag{A71}$$

It can also be shown that

$$\gamma_{n-1} = \int_{-1}^{1}(1-x^2)\left(P'_{n-1}(x)\right)^2\mathrm{d}x = \frac{2n(n-1)}{2n-1} \tag{A72}$$

Employing these values for a_{n-1} and γ_{n-1} in equation A67 we have

$$\int_{-1}^{1}\frac{(1-x^2)P'_{n-1}(x)}{x-x_i}\mathrm{d}x = \frac{2n}{P'_n(x_i)} \tag{A73}$$

which is precisely equation A63, which we initially set out to prove, and we are left with the equation

$$w_i = -\frac{2n}{(1 - x_i^2)P''_{n-1}(x_i)P'_n(x_i)} \tag{A74}$$

for the interior integration weights.

This concludes the derivation of the Lobatto Quadrature.

Appendix B: Integration Methods for the DAF Operators

A crucial step in the DAF process is the accurate numerical evaluation of the convolution integrals. In the case where the functions in question have compact support, that is, they go to zero at $x \to \pm\infty$.