Advanced Computational Fluid Dynamics
AA215A Lecture 3
Polynomial Interpolation: Numerical Differentiation and Integration

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Winter Quarter, 2016, Stanford, CA
Last revised on January 7, 2016

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Lecture 3

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3.1 Interpolation Polynomials

So far we have not required $P_n(x)$ to equal $f(x)$ at any points in the interval. This permits some smoothing! A natural approach is to make $P_n(x) = a_0 + a_1x + ... + a_nx^n = f(x)$ at $n+1$ points $x_0, x_1, ..., x_n$. Then we have $n+1$ equations for the $n+1$ coefficients. Such a polynomial is called an interpolation polynomial. A solution exists because the determinant of the equations is the Vandemonde determinant

$$D = \begin{vmatrix} 1 & x_0 & ... & x_0^n \\ 1 & x_1 & ... & x_1^n \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & ... & x_n^n \end{vmatrix} = \prod_{i>j}(x_i - x_j) \neq 0 \tag{3.1}$$

This can be seen by noting that D vanishes if any x_i equals any x_j, but D is a polynomial of just the same order as the product. The interpolation polynomial is unique since if there were 2 such polynomials $P_n(x), Q_n(x)$, then

$$P_n(x_i) - Q_n(x_i) = 0 \text{ for } i = 0, 1, ..., n \tag{3.2}$$

But then $P_n(x) - Q_n(x)$ is an n^{th} degree polynomial with $n+1$ roots, so it must be zero.

In practice it is easiest to construct $P_n(x)$ indirectly as a sum of specially chosen polynomials rather than solve for the a_j. To do this note that

$$\phi_{n,j}(x) = \frac{(x-x_0)(x-x_1)...(x-x_{j-1})(x-x_{j+1})...(x-x_n)}{(x_j-x_0)(x_j-x_1)...(x_j-x_{j-1})(x_j-x_{j+1})...(x_j-x_n)} = 1 \text{ when } x = x_j \tag{3.3}$$

Then we can get

$$P_n(x) = \sum_{j=0}^{n} f(x_j)\phi_{n,j}(x) \tag{3.4}$$

which equals $f(x)$ at $x = x_0, x_1, ..., x_n$, and is the only such polynomial as has just been shown.

The $\phi_{n,j}(x)$ are called Lagrange interpolation coefficients. We can write

$$\phi_{n,j}(x) = \frac{w_n(x)}{(x-x_j)w_n'(x_j)} \tag{3.5}$$

where

$$w_n(x) = (x - x_0)(x - x_1)...(x - x_n) \tag{3.6}$$

3.2 Error in the Interpolating Polynomial

We shall show that if $f(x)$ has an $(n+1)^{\text{th}}$ derivative and $P_n(x)$ is an interpolating polynomial then the remainder is

$$f(x) - P_n(x) = \frac{(x - x_0)(x - x_1)...(x - x_n)}{(n+1)!} f^{(n+1)}(\xi) \tag{3.7}$$

where ξ is in the interval defined by $x_0, x_1, ..., x_n$.

Let $S_n(x)$ be defined by

$$f(x) - P_n(x) = w_n(x) S_n(x) \tag{3.8}$$

where

$$w_n(x) = (x - x_0)(x - x_1)...(x - x_n) \tag{3.9}$$

Define

$$F(z) = f(z) - P_n(z) - w_n(z) S_n(x) \tag{3.10}$$

This is continuous in z and vanishes at $n+2$ points $x_0, x_1, ..., x_n, x$. Thus by Rolle's theorem $F'(z)$ vanishes at $n+1$ points, $F''(z)$ vanishes at n points, ..., and finally $F^{(n+1)}(z)$ vanishes at one point ξ. But

$$\frac{d^{n+1}}{dz^{n+1}} P_n(z) = 0 \tag{3.11}$$

$$\frac{d^{n+1}}{dz^{n+1}} w_n(z) S_n(x) = (n+1)! S_n(x) \tag{3.12}$$

Thus

$$F^{(n+1)}(z) = f^{n+1}(z) - (n+1)! S_n(x) \tag{3.13}$$

and setting $z = \xi$

$$S_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi) \tag{3.14}$$

$$f(x) - P_n(x) = \frac{w_n(x)}{(n+1)!} f^{(n+1)}(\xi) \tag{3.15}$$

Since the error depends on $w_n(x)$ we naturally ask how the x_i should be distributed to minimize $w_n(x)$.

3.3 Error of Derivative with Lagrange Interpolation

Suppose that

$$f(x) = P_n(x) + \frac{w_n}{(n+1)!} f^{(n+1)}(\xi) \tag{3.16}$$

Then

$$f'(x) = P_n'(x) + \frac{w_n'}{(n+1)!} f^{(n+1)}(\xi) + \frac{w_n}{(n+1)!} f^{(n+2)}(\xi) \frac{d\xi}{dx} \tag{3.17}$$

where

$$w_n' = \sum_{j=0}^{n} \prod_{k \neq j}^{n} (x - x_k) \tag{3.18}$$

Then at an interpolation point,

$$f'(x_j) = P_n'(x_j) + \prod_{k \neq j}^{n} (x_j - x_k) \frac{f^{(n+1)}}{(n+1)!}(\xi) \tag{3.19}$$

with equal intervals h

$$f'(x_0) = P'(x_0) + \frac{h^n}{n+1} f^{(n+1)}(\xi) \tag{3.20}$$

since

$$(x_1 - x_0)(x_2 - x_0)...(x_n - x_0) = n!h^n \tag{3.21}$$

With one interval,

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} + \frac{h}{2} f''(\xi) \tag{3.22}$$

3.4 Error of the k^{th} Derivative of the Interpolation Polynomial

Let $f^{n+1}(x)$ be continuous and let

$$R_n(x) = f(x) - P_n(x) \tag{3.23}$$

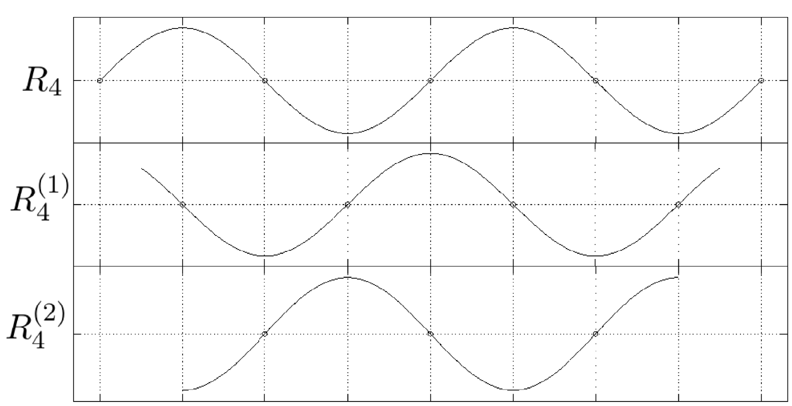
Then

$$R_n^{(k)}(x) = \prod_{j=0}^{n-k} (x - \xi_j) \frac{f^{(n+1)}(\xi)}{(n+1-k)!} \tag{3.24}$$

where the distinct points ξ_j are independent of x and lie in the intervals $x_j < \xi_j < x_{j+k}$ for $j = 0, 1, ..., n-k$ and $\xi(x)$ is some point in the interval containing x and the ξ_j.

Proof:

$R_n = f - P_n$ has $n+1$ continuous derivatives and vanishes at $n+1$ points $x = x_j$, for $j = 0, 1, ..., n$. Apply Rolle's theorem $k \leq n$ times. The zeros are then distributed as illustrated.



This leads to the following table for the distribution of the $n-k+1$ zeros ξ_j of $R_n^{(k)}$.

R	$R^{(1)}$	$R^{(2)}$	$\cdots$	$R^{(k)}$
x_0				
x_1	(x_0, x_1)			
x_2	(x_1, x_2)	(x_0, x_2)		
$\vdots$				
x_k	(x_{k-1}, x_k)	(x_{k-2}, x_k)	$\cdots$	(x_0, x_k)
$\vdots$				
x_n	(x_{n-1}, x_n)	(x_{n-2}, x_n)	$\cdots$	(x_{n-k}, x_n)

Define

$$F(z) = R_n^{(k)}(z) - \alpha \prod_{j=0}^{n-k} (z - \xi_j) \tag{3.25}$$

For any x distinct from the ξ_j choose α such that

$$F(x) = 0 \tag{3.26}$$

Then $F(z)$ has $n-k+2$ zeros and by Rolle's theorem $F^{(n-k+1)}(z)$ has one zero, η, say, in the interval containing x and the ξ_j.
Thus

$$\begin{aligned} 0 &= F^{(n-k+1)}(\eta) && (3.27) \\ &= R_n^{n+1}(\eta) - \alpha(n-k+1)! && (3.28) \\ &= f^{n+1}(\eta) - \alpha(n-k+1)! && (3.29) \end{aligned}$$

or

$$\alpha = \frac{f^{n+1}(\eta)}{(n-k+1)!} \tag{3.30}$$

It follows that for a mesh width bounded by h

$$R_n^{(k)} \leq M h^{n-k+1} \tag{3.31}$$

where M is proportional to $\sup \left| f^{n+1}(x) \right|$ in the interval.

3.5 Interpolation with a Triangle of Polynomials

Set

$$\begin{aligned} w_0(x) &= (x - x_0) \\ w_1(x) &= (x - x_0)(x - x_1) \\ w_k(x) &= (x - x_0)(x - x_1)...(x - x_k) \end{aligned}$$

Now to interpolate $f(x)$ with values f_i at x_i we set

$$p(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1)... \tag{3.32}$$

Then

$$\begin{aligned} p_0(x_0) &= f_0 = a_0 \\ p_1(x_1) &= f_1 = a_0 + a_1(x_1 - x_0) \\ p_2(x_2) &= f_2 = a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1) \\ &\vdots \end{aligned}$$

so we can solve for the a_i in succession

$$a_k = \frac{f_k - a_0 - a_1(x_k - x_0) - ... - a_{k-1}(x_k - x_0)...(x_k - x_{k-2})}{(x_k - x_0)(x_k - x_1)...(x_k - x_{k-1})} = \frac{f_k - p_{k-1}(x_k)}{w_{k-1}(x_k)} \tag{3.33}$$

3.6 Newton's Form of the Interpolation Polynomial

The Lagrangian form of the interpolation polynomial has the disadvantage that the coefficients have to be recomputed if a new interpolation point is added. To avoid this let

$$P_n(x) = \sum_{k=0}^{n} a_k w_{k-1}(x) \tag{3.34}$$

where

$$w_k(x) = (x - x_0)(x - x_1)...(x - x_k) \text{ and } w_{-1}(x) = 1 \tag{3.35}$$

We can determine the a_k so that

$$P_n(x_j) = f(x_j) \text{ for } j = 0, 1, ..., n \tag{3.36}$$

Suppose this has been done for P_{k-1}, and we now add x_k. Then

$$P_k(x) = P_{k-1}(x) + a_k w_{k-1}(x) \tag{3.37}$$

$$P_k(x_j) = P_{k-1}(x_j) = f(x_j) \text{ for } j = 0, 1, ..., k-1 \tag{3.38}$$

$$P_k(x_k) = P_{k-1}(x_k) + a_k w_{k-1}(x_k) = f(x_k) \tag{3.39}$$

where $a_k = \frac{f(x_k) - P_{k-1}(x_k)}{w_{k-1}(x_k)}$.

On the other hand the coefficient of the highest order term in the Lagrange expression is

$$\sum_{j=0}^{n} \frac{f(x_j)}{w_n'(x_j)} \tag{3.40}$$

so by comparison

$$a_n = \sum_{j=0}^{n} \frac{f(x_j)}{w_n'(x_j)} \tag{3.41}$$

Thus a_n is a linear combination of $f(x_j)$ for $j = 0, 1, ..., n$. Multiply by

$$x_n - x_0 = x_n - x_j + x_j - x_0 \tag{3.42}$$

Then

$$\begin{aligned} a_n(x_n - x_0) &= -\sum_{j=0}^{n} \frac{f(x_j)}{w'_n(x_j)}(x_j - x_n) + \sum_{j=1}^{n} \frac{f(x_j)}{w'_n(x_j)}(x_j - x_0) \\ &= -\sum_{j=0}^{n} \frac{f(x_j)}{\prod_{k\neq j}(x_j - x_k)} + \sum_{j=1}^{n} \frac{f(x_j)}{\prod_{k\neq j}(x_j - x_k)} \end{aligned} \tag{3.43}$$

These are just the expressions for a_{n-1} in the intervals x_0 to x_{n-1} and x_1 to x_n. Thus if we define

$$f[x_0, ..., x_n] = a_n = \sum_{j=0}^{n} \frac{f(x_j)}{\prod_{k\neq j}(x_j - x_k)} \tag{3.44}$$

we find that

$$f[x_0, ..., x_n](x_0 - x_n) = f[x_1, ..., x_n] - f[x_0, ..., x_{n-1}] \tag{3.45}$$

and starting from

$$f[x_0] = f(x_0) \tag{3.46}$$

we have

$$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0} \tag{3.47}$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} \tag{3.48}$$

giving Newton's form of the interpolation polynomial

$$P_n(x) = f[x_0] + (x - x_0)f[x_0, x_1] + ... + (x - x_0)...(x - x_{n-1})f[x_0, ..., x_n] \tag{3.49}$$

The square bracketed expressions are Newton's divided differences, and we now have Newton's form for the interpolation polynomial:

$$P_n(x) = f[x_0] + (x - x_0)f[x_0, x_1] + ... + (x - x_0)...(x - x_{n-1})f[x_0, ..., x_n] \tag{3.50}$$

where each new term is independent of the previous terms.

To estimate the magnitude of the higher divided differences we can use the result already obtained for the remainder.

Theorem: Let $x_0, x_1, ..., x_{k-1}$ be distinct points and let f be continuous in interval containing all these points. Then for some point ξ in this interval

$$f[x_0, ..., x_{k-1}, x] = \frac{f^{(k)}(\xi)}{k!} \tag{3.51}$$

Proof: From Newton's formula

$$f(x) - P_{k-1}(x) = (x - x_0)...(x - x_{k-1})f[x_0, ..., x_{k-1}, x] = (x - x_0)...(x - x_{k-1})\frac{f^{(k)}(\xi)}{k!} \tag{3.52}$$

by the remainder theorem. But x is distinct from $x_0, x_1, ..., x_{k-1}$ so the theorem follows on dividing out the factors.

3.7 Hermite Interpolation

We can generalize interpolation by matching derivatives as well as values at the interpolation points. Such a polynomial is called the osculating polynomial and the procedure is called Hermite interpolation.

Let $H_{2n+1}(x)$ be a polynomial of degree $2n+1$ such that

$$H_{2n+1}(x) = f(x_j) \text{ for } j = 0, 1, ..., n \tag{3.53}$$

$$H'_{2n+1}(x) = f'(x_j) \text{ for } j = 0, 1, ..., n \tag{3.54}$$

The $2n+2$ coefficients are needed to satisfy $2n+2$ conditions. $H_{2n+1}(x)$ can be found indirectly as in Lagrange interpolation.

Let $\psi_{n,j}(x)$ and $\gamma_{n,j}(x)$ be polynomials of degree $2n+1$ such that

$$\begin{array}{ll} \psi_{n,j}(x_i) = \delta_{ij}, \;\; \psi'_{n,j}(x_i) = 0, & \text{for } i = 0, 1, ..., n \\ \gamma_{n,j}(x_i) = 0 \quad , \;\; \gamma'_{n,j}(x_i) = \delta_{ij}, & \text{for } i = 0, 1, ..., n \end{array}$$

Then the Hermite interpolation polynomial is

$$H_{2n+1}(x) = \sum_{j=0}^{n} \left(f(x_j)\psi_{n,j}(x) + f'(x_j)\gamma_{n,j}(x) \right) \tag{3.55}$$

It can be directly verified by differentiation that the required polynomials are

$$\psi_{n,j}(x) = (1 - 2\phi'_{n,j}(x)(x - x_j))\phi^2_{n,j}(x) \tag{3.56}$$

and

$$\gamma_{n,j}(x) = (x - x_j)\phi^2_{n,j}(x) \tag{3.57}$$

where $\phi_{n,j}(x)$ are the Lagrange polynomials satisfying

$$\phi_{n,j}(x_i) = \delta_{ij} \text{ for } i = 0, 1, ..., n \tag{3.58}$$

The error in Hermite interpolation is

$$f(x) - H_{2n+1}(x) = \omega^2_n(x)\frac{f^{2n+2}(\xi)}{(2n+2)!} \tag{3.59}$$

where

$$\omega_n(x) = (x - x_0)(x - x_1)...(x - x_n) \tag{3.60}$$

This can be proved in the same way as the error estimate for Lagrange interpolation where now

$$F(\xi) = f(\xi) - H_{2n+1}(\xi) - \omega^2_n(\xi)S_n(x) \tag{3.61}$$

and on the first application of Rolle's theorem $F'(\xi)$ has $2n+2$ distinct zeros.

The Hermite polynomial can be obtained via a passage to the limit from the Lagrange polynomial $P_{2n+1}(x)$ which interpolates $f(x)$ at the $2n+2$ points

$$x_0, x_0 + h, x_1, x_1 + h, ..., x_n, x_n + h \tag{3.62}$$

as $h \to 0$ to produce $n+1$ pairs of coincident points. Define

$$N(h) = \prod_{k=1,n,\quad k\neq j} (x - x_k + h) \tag{3.63}$$

and

$$D(h) = \prod_{k=1,n,\quad k\neq j} (x_j - x_k + h) \tag{3.64}$$

Then the contribution of the points x_j and $x_j + h$ to $P_{2n+1}(x)$ is

$$\begin{aligned} Q(x) &= f(x_j)\frac{N(0)}{D(0)}\frac{N(-h)}{D(-h)}\frac{x-(x_j+h)}{x_j-(x_j+h)} \\ &+ f(x_j+h)\frac{N(0)}{D(h)}\frac{N(-h)}{D(0)}\frac{x-x_j}{h} \end{aligned}$$

Expanding $f(x_j+h)$ in a Taylor series

$$\begin{aligned} Q(x) &= f(x_j)\frac{N(0)}{D(0)}\frac{N(-h)}{D(-h)}\frac{x-(x_j+h)}{x_j-(x_j+h)} \\ &+ \left(f(x_j)+hf'(x_j)+O(h^2)\right)\frac{N(0)}{D(h)}\frac{N(-h)}{D(0)}\frac{x-x_j}{h} \\ &= f(x_j)\frac{N(0)}{D(0)}\left[\frac{N(-h)}{D(-h)} - \frac{x-x_j}{h}N(-h)\left(\frac{1}{D(-h)}-\frac{1}{D(h)}\right)\right] \\ &+ f'(x_j)(x-x_j)\frac{N(0)}{D(0)}\frac{N(-h)}{D(h)} + O(h) \end{aligned}$$

Also

$$\frac{1}{D(-h)} - \frac{1}{D(h)} = 2h\frac{D'(0)}{D^2(0)} + O(h^2) \tag{3.65}$$

Thus in the limit as $h \to 0$

$$\begin{aligned} Q(x) &= f(x_j)\frac{N^2(0)}{D^2(0)}\left(1 - 2(x-x_j)\frac{D'(0)}{D(0)}\right) \\ &+ f'(x_j)(x-x_j)\frac{N^2(0)}{D^2(0)} \end{aligned}$$

where

$$\frac{N(0)}{D(0)} = \phi_{n,j}(x) \tag{3.66}$$

and $D'(0)$ equals $\frac{d}{dx}N(0)$ evaluated at x_j, so that

$$\frac{D'(0)}{D(0)} = \phi'_{n,j}(x_j) \tag{3.67}$$

3.8 Integration Formulas using Polynomial Interpolation

Let $P_{n-1}(x)$ interpolate $f(x)$ at $x_0, x_1, ..., x_n$. Then

$$P_n(x) = \sum_{j=0}^{n} f(x_j)\phi_{n,j}(x) \tag{3.68}$$

where

$$\phi_{n,j}(x) = \frac{\prod_{k\neq j}(x - x_k)}{\prod_{k\neq j}(x_j - x_k)} \tag{3.69}$$

so that

$$\phi_{n,j}(x_k) = \delta_{jk} \tag{3.70}$$

Now approximate $\int_a^b f(x)dx$ by $\int_a^b P_n(x)dx$ where typically $a = x_0, b = x_n$. Then

$$\int_a^b f(x)dx = \sum_{j=0}^{n} A_j f(x_j) + E(f) \tag{3.71}$$

where $E(f)$ denotes the error, and

$$A_j = \int_a^b \phi_{n,j}(x)dx \tag{3.72}$$

The result is exact if $f(x)$ is a polynomial of degree $\leq n$, since then $P_n(x) = f(x)$. This is called precision of degree n.

3.9 Integration with a weight function

We may include a weight function $w(x) \geq 0$ in the integral. Then

$$\int_a^b f(x)w(x)dx = \sum_{j=n}^{n} A_j f(x_j) + E(f) \tag{3.73}$$

where now

$$A_j = \int_a^b \phi_{n,j}(x)w(x)dx \tag{3.74}$$

Depending on $w(x)$, analytical expressions are not necessarily available for evaluating the coefficients A_j.

3.10 Newton Cotes formulas

These are derived by approximating $f(x)$ by an interpolation formula using $n + 1$ equally spaced points in $[a, b]$ including the end points. The first 3 such formulas are:
Trapezoidal rule

$$\int_a^b f(x)dx = \frac{h}{2}(f(a) + f(b)) + E(f),\ h = b - a \tag{3.75}$$

Simpson's rule

$$\int_a^b f(x)dx = \frac{h}{3}f(a) + \frac{4h}{3}f(a+h) + \frac{h}{3}f(b) + E(f),\ h = \frac{b-a}{2} \tag{3.76}$$

and Simpson's $\frac{3}{8}$ formula

$$\int_a^b f(x)dx = \frac{3h}{8}f(a) + \frac{9h}{8}f(a+h) + \frac{9h}{8}f(a+2h) + \frac{3h}{8}f(b) + E(f),\ h = \frac{b-a}{3} \tag{3.77}$$

3.11 Gauss Quadrature

When the interpolation points x are fixed the integration formula has $n+1$ degrees of freedom corresponding to the coefficients A_j for $j = 0, ..., n$. Accordingly we can find values of A_j which yield exact values of the integral of all polynomials of degree n,

$$P_n(x) = a_0 + a_1 x + ... + a_n x^n, \tag{3.78}$$

since these also have $n+1$ degrees of freedom corresponding to the coefficients a_j for $j = 0, ..., n$. If we are also free to choose the integration points x_j, then we have $2n+2$ degrees of freedom corresponding to x_j and A_j, for $j = 0, ..., n$. Now it is possible to find values of x_j and A_j which enable exact integration of polynomials of degree $\leq 2n+1$. One could try to find the required values by solving $2n+2$ nonlinear equations

$$\sum_{j=0}^{n} A_j f(x_j) = \int_a^b f(x)dx \tag{3.79}$$

where $f(x) = 1, x, ..., x^{2n+1}$ in turn. However the required values can be found indirectly as follows.

Let $\phi_i(x)$ be orthogonal polynomials for the weight function $w(x)$, so that

$$\int_a^b \phi_j(x)\phi_k(x)w(x) = 0 \text{ for } j \neq k \tag{3.80}$$

Choose x_j as the zeros of $\phi_{n+1}(x)$. Then integration using polynomial interpolation is exact for polynomials up to degree $2n+1$.

Proof:

If $f(x)$ is a polynomial of degree $\leq 2n+1$ it can be uniquely expressed as

$$f(x) = q(x)\phi_{n+1}(x) + R(x) \tag{3.81}$$

where $q(x)$ and $R(x)$ are polynomials of degree $\leq n$. Then

$$\int_a^b f(x)w(x)dx = \int_a^b q(x)\phi_{n+1}(x)w(x)dx + \int_a^b R(x)w(x)dx = \int_a^b R(x)w(x)dx \tag{3.82}$$

since $\phi_{n+1}(x)$ is orthogonal to all polynomials of degree $< n+1$.

Also the approximate integral is

$$\begin{aligned} I &= \sum_{j=0}^{n} A_j f(x_j) \\ &= \sum_{j=0}^{n} A_j q(x_j)\phi_{n+1}(x_j) + \sum_{j=0}^{n} A_j R(x_j) \\ &= \sum_{j=0}^{n} A_j R(x_j) \end{aligned} \tag{3.83}$$

since $\phi_{n+1}(x_j)$ is zero for $j = 0, 1, ..., n$. But then

$$I = \int_a^b R(x)w(x)dx \tag{3.84}$$

exactly, since $R(x)$ is a polynomial of degree $\leq n$.

The degree of precision $2n+1$ is the maximum attainable. Consider the polynomial of $\phi_{n+1}^2(x)$ of degree $2n+2$. Then

$$I = 0 \tag{3.85}$$

since $\phi_{n+1}(x_j) = 0$ for $j = 0, 1, ..., n$. But

$$\int_a^b \phi_{n+1}^2(x)w(x)dx > 0 \tag{3.86}$$

because $\phi_{n+1}^2(x) > 0$ except at the zeros $x_0, x_1, ..., x_n$.

When applied to an arbitrary smooth function $f(x)$ which can be expanded as

$$f(a) + (x-a)f'(a) + ... + \frac{(x-a)^{2n+2}}{(2n+2)!} f^{(2n+2)}(\xi) \tag{3.87}$$

the error is proportional to a bound on $|f^{(2n+2)}(x)|$ because the preceding terms in the Taylor series are integrated exactly.

3.12 Formulas for Gauss integration with constant weight function

Number of Points	x_j	A_j	Precision	Order
1	0	2	1	2
2	$\pm\frac{1}{\sqrt{3}}$	1	3	4
3	0 $\pm\frac{\sqrt{15}}{5}$	$\frac{8}{9}$ $\frac{5}{9}$	5	6
4	$\pm\frac{\sqrt{3-2\sqrt{\frac{6}{5}}}}{7}$ $\pm\frac{\sqrt{3+2\sqrt{\frac{6}{5}}}}{7}$	$\frac{18+\sqrt{30}}{36}$ $\frac{18-\sqrt{30}}{36}$	7	8
5	0 $\pm\sqrt{5-2\sqrt{\frac{10}{7}}}$ $\pm\sqrt{5+2\sqrt{\frac{10}{7}}}$	$\frac{128}{225}$ $\frac{322+13\sqrt{70}}{900}$ $\frac{322-13\sqrt{70}}{900}$	9	10

Table 3.1: Formulas for Gauss integration with constant weight function

3.13 Error bound for Gauss integration

Let $H_{2n+1}(x)$ be the Hermite interpolation polynomial to $f(x)$ at the integration points. The Gauss integration formula is exact for $H_{2n+1}(x)$. Hence

$$\int_a^b H_{2n+1}(x)w(x)dx = \sum_{j=0}^{n} A_j Q(x_j) = \sum_{j=0}^{n} A_j f_j \tag{3.88}$$

Thus

$$\int_a^b f(x)w(x)dx - \sum_{i=0}^{n} A_j f_j = \int_a^b (f(x) - H_{2n+1}(x))w(x)dx \tag{3.89}$$

According to the error formula for Hermite interpolation

$$f(x) - H_{2n+1}(x) = \tilde{P}_n^2(x)\frac{f^{(2n+2)(\xi)}}{(2n+2)!} \tag{3.90}$$

where

$$\tilde{P}_n(x) = (x-x_0)(x-x_1)...(x-x_n) \tag{3.91}$$

is the orthogonal polynomial normalized so that its leading coefficient is unity.

Then the error is

$$E = \frac{1}{(2n+2)!}\int_a^b w(x)\tilde{P}_n^2(x)f^{(2n+2)}(\xi)dx \tag{3.92}$$

Since $w(x)\hat{P}_n^2(x) \geq 0$ the error lies in the range between

$$\min f^{(2n+2)}(\xi)A \quad \text{and} \quad \max f^{(2n+2)}(\xi)A \tag{3.93}$$

where

$$A = \frac{1}{(2n+2)!} \int_a^b w(x) \tilde{P}_n^2(x) dx \tag{3.94}$$

and hence

$$E = A f^{(2n+2)}(\eta) \tag{3.95}$$

for some value of η in $[a, b]$.

3.14 Discrete orthogonality of orthogonal polynomials

Let $\phi_j(x)$ be orthogonal polynomials satisfying

$$(\phi_j, \phi_k) = \int_a^b \phi_j(x)\phi_k(x)w(x)dx = 0 \text{ for } j \neq k \tag{3.96}$$

Let x_i be the zeros of $\phi_{n+1}(x)$.

Then if $j \leq n, k \leq n$, $\phi_j(x)\phi_k(x)$ is a polynomial of degree $\leq 2n$. Accordingly (ϕ_j, ϕ_k) is evaluated exactly by Gauss integration. This implies that the ϕ_j satisfy the discrete orthogonality condition

$$\sum_{i=0}^{n} A_i \phi_j(x_i)\phi_k(x_i) = 0, \text{ given } j \neq k, j \leq n, k \leq n \tag{3.97}$$

where A_i are the coefficients for Gauss integration at the zeros of ϕ_{n+1}.

3.15 Equivalence of interpolation and least squares approximation using Gauss integration

Let $f^*(x)$ be the least squares fit to $f(x)$ using orthogonal polynomials $\phi_j(x)$ for the interval $[a, b]$ with weight function $w(x) \geq 0$. Then

$$f^*(x) = \sum_{j=0}^{n} c_j^* \phi_j(x) \tag{3.98}$$

where

$$c_j^* = \frac{(f, \phi_j)}{(\phi_j, \phi_j)} = \frac{\int_a^b f(x)\phi_j(x)w(x)dx}{\int_a^b \phi_j^2(x)w(x)dx} \tag{3.99}$$

Let x_i be the zeros of $\phi_{n+1}(x)$, and let $P_n(x)$ be the interpolation polynomial to $f(x)$ satisfying

$$P_n(x_i) = f(x_i) \text{ for } i = 0, 1, ..., n \tag{3.100}$$

$P_n(x)$ can be expanded as

$$P_n(x) = \sum_{k=0}^{n} \hat{c}_k \phi_k(x) \tag{3.101}$$

Then the $\hat{c}_k$ are determined by the conditions

$$\sum_{k=0}^{n} \hat{c}_k \phi_k(x_i) = f(x_i) \text{ for } i = 0, 1, ..., n \tag{3.102}$$

Also the polynomials $\phi_j(x)$ satisfy the discrete orthogonality condition

$$\sum_{i=0}^{n} A_i \phi_j(x_i)\phi_k(x_i) = 0 \text{ given } j \neq k, j \leq n, k \leq n \tag{3.103}$$

where A_i are the coefficients for Gauss integration.

Now multiplying (3.102) by $A_i\phi_j(x_i)$ and summing over i, it follows that

$$\hat{c}_j = \frac{\sum_{i=0}^{n} A_i f(x_i)\phi_j(x_i)}{\sum_{i=0}^{n} A_i \phi_j^2(x_i)} \tag{3.104}$$

This is exactly the formula (3.99) for evaluating the least squares coefficient c_j^* by Gauss integration.
Alternative Proof:
The coefficients $\hat{c}_j$ are actually the least squares coefficients which minimize

$$J = ||f - \sum_{j=0}^{n} c_j \phi_j||^2 \tag{3.105}$$

in the discrete semi-norm in which

$$\int \left(f(x) - \sum_{j=0}^{n} c_j \phi_j(x) \right)^2 w(x)dx \tag{3.106}$$

is evaluated by Gauss integration at the zeros x_i of $\phi_{n+1}(x)$ as

$$J = \sum_{i=0}^{n} A_i \left(f(x_i) - \sum_{j=0}^{n} c_j \phi_j(x_i) \right)^2 w(x_0) \tag{3.107}$$

But as a consequence of the interpolation condition (3.99) the coefficients $\hat{c}_j$ yield the value $J = 0$, thus minimizing J.

3.16 Gauss Lobato Integration

To integrate $f(x)$ over [-1,1] choose integration points at $-1, 1$, and the zeros of Q_{n-1}, which are the zeros of

$$(1 + x)(1 - x)\phi_{n-1}(x) \tag{3.108}$$

Then let

$$f(x) = q(x)(1 - x^2)\phi_{n-1}(x) + r(x) \tag{3.109}$$

where if $f(x)$ is a polynomial of degree $\leq 2n - 1$, $q(x)$ and $r(x)$ are polynomial of degree $\leq n - 2$.
Now let the polynomials ϕ_j be orthogonal for the weight function

$$w(x) = 1 - x^2 \tag{3.110}$$

Then

$$I = \int_{-1}^{1} f(x)dx = \int_{-1}^{1} q(x)\phi_{n-1}(x)w(x)dx + \int_{-1}^{1} r(x)dx = \int_{-1}^{1} r(x)dx \tag{3.111}$$

since ϕ_{n-1} is orthogonal to all polynomials of lower degree. Also the approximate integral is

$$\hat{I} = \sum_{j=0}^{n} A_j f(x_j) \tag{3.112}$$

where

$$A_j = \int_{-1}^{1} \phi_{n,j}(x) dx \tag{3.113}$$

Then

$$\hat{I} = \sum_{j=0}^{n} A_j q(x_j)(1 - x_j^2)\phi_{n-1}(x_j) + \sum_{j=0}^{n} A_j r(x_j) = \sum_{j=0}^{n} A_j r(x_j) \tag{3.114}$$

since $(1 - x_j^2)\phi_{n-1}(x_j) = 0$ for $j = 0, 1, ..., n$. But then

$$\hat{I} = I \tag{3.115}$$

since $r(x)$ is a polynomial of degree $< n$. Here ϕ_j are the Jacobi polynomials $P_j^{(1,1)}$, where $P_j^{(\alpha,\beta)}$ is orthogonal for the weight

$$(1 - x)^{\alpha}(1 + x)^{\beta} \tag{3.116}$$

3.17 Portraits of Lagrange, Newton and Gauss

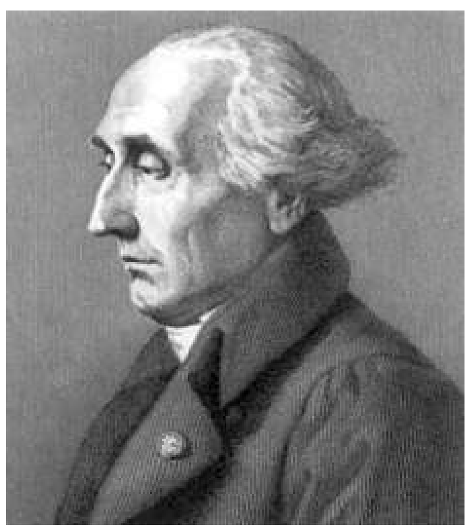


Figure 3.1: Joseph-Louis Lagrange (1736-1813)

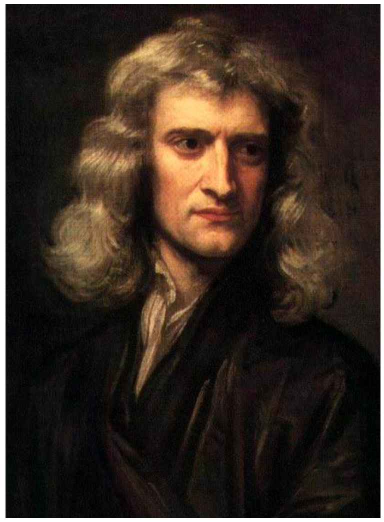


Figure 3.2: Sir Isaac Newton (1642-1726)

Figure 3.3: Carl Friedrich Gauss (1777-1855)