Review We have constructed the Newton formula for Lagrange interpolation:

$$p_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + \cdots + f[x_0, \ldots, x_n](x - x_0)(x - x_1)\cdots(x - x_{n-1})$$

is the degree-n polynomial p_n satisfying $p_n(x_j) = f_j$ for $0 \leq j \leq n$. Here $f[x_j] = f(x_j)$ and

$$f[x_0, \ldots, x_k] = \frac{f[x_1, \ldots, x_k] - f[x_0, \ldots, x_{k-1}]}{x_k - x_0}.$$

(A consequence is the symmetry of divided differences: every divided difference is independent of the ordering of the interpolation points.) The error satisfies

$$f(x) - p_n(x) = \frac{1}{(n+1)!} f^{(n+1)}(\xi)\omega(x)$$

where ξ is some unknown point contained in the interval $[\min x_j, \max x_j]$ and

$$\omega(x) = (x - x_0)(x - x_1)\cdots(x - x_n).$$

Differences and derivatives The Newton formula makes it simple to add $x_{n+1} = x$ as an additional interpolation point, and the value $p_{n+1}(x) = f(x)$ is then exact:

$$f(x) = p_{n+1}(x) = p_n(x) + f[x_0, x_1, \ldots, x_{n-1}, x_n]\omega(x)$$

Comparing with the error formula proves a theorem: every divided difference is proportional to a derivative

$$f[x_0, x_1, \ldots, x_n] = \frac{f^{(n+1)}(\xi)}{(n+1)!},$$

evaluated at some unknown point ξ contained in the interval $[\min x_j, \max x_j]$. This proportionality is important because as the interpolation points x_j coalesce into a single point x, they trap the unknown evaluation point ξ between them:

$$f[x_0, x_1, \ldots, x_n] \to \frac{f^{(n+1)}(x)}{(n+1)!}$$

as all the x_j's approach x. So Newton's formula has a limit as interpolation points coalesce. If the x_j's all coalesce into a single point x, Newton's interpolation formula becomes a Taylor expansion for the Taylor polynomial which matches as many derivatives as it can with f at x. For example, if $n = 0$ then the linear interpolant

$$p(x) = f[x_0] + f[x_0, x_1](x - x_0)$$

has a limit as $x_1 \to x_0$ because

$$f[x_0, x_1] \to f'(x_0) = f_0'$$

as $x_1 \to x_0$. Thus

$$p(x) = f[x_0] + f[x_0, x_0](x - x_0) = f(x_0) + f'(x_0)(x - x_0)$$

reproduces the first-order Taylor expansion.

Hermite interpolation bridges Lagrange interpolation and Taylor expansion by matching selected derivatives as well as function values at selected points. For example, let's find a degree $2n+1$ polynomial $p(x)$ with

$$p(x_j) = f_j$$

and

$$p'(x_j) = f'_j$$

for $0 \le j \le n$. Newton's formula makes this easy. With two points we want

$$p(x_j) = f_j$$

and

$$p'(x_j) = f'_j.$$

We build up p gradually

$$p(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)^2 + a_3(x - x_0)^2(x - x_1)$$

choosing each a_j so that the previously satisfied interpolation conditions remain satisfied. To do this, build the difference table

x	$f[1]$	$f[2]$	$f[3]$	$f[4]$
x_0	f_0	$a_1 = f'_0$	$a_2 = f[x_0, x_0, x_1]$	a_3
x_0	f_0	$f[x_0, x_1]$	$a_2 = f[x_0, x_1, x_1]$	
x_1	f_1	f'_1		
x_1	f_1			

Repeat x values as many times as derivatives are to be specified. Substitute derivatives divided by factorials whenever divide by zero would otherwise occur.

For example, with $f(x) = 2^x$ so $f'(x) = (\log 2)2^x$ we build a cubic interpolant to f and f' at $x_0 = 0$ and $x_1 = 1$ with the table

x	$f[1]$	$f[2]$	$f[3]$	$f[4]$
0	1	$\log 2$	$1 - \log 2$	$3\log 2 - 2$
0	1	1	$2\log 2 - 1$	
1	2	$2\log 2$		
1	2			

so

$$p(x) = 1 + (\log 2)x + (1 - \log 2)x^2 + (3\log 2 - 2)x^2(x - 1)$$

is the Hermite interpolant in Newton form.

If we want to add a new interpolation point $x_2 = 2$, we just add two diagonals to the table and two terms to p:

x	$f[1]$	$f[2]$	$f[3]$	$f[4]$	$f[5]$	$f[6]$
0	1	$\log 2$	$1 - \log 2$	$3\log 2 - 2$	$(5 - 5\log 2)/2$	$(13\log 2 - 11)/4$
0	1	1	$2\log 2 - 1$	$3 - 2\log 2$	$(8\log 2 - 6)/2$	
1	2	$2\log 2$	$2 - 2\log 2$	$6\log 2 - 3$		
1	2	2	$4\log 2 - 1$			
2	4	$4\log 2$				
2	4					

and

$$p(x) = 1 + (\log 2)x + (1 - \log 2)x^2 + (3\log 2 - 2)x^2(x-1)$$
$$+((5 - 5\log 2)/2)x^2(x-1)^2 + ((13\log 2 - 11)/4)x^2(x-1)^2(x-2)$$

is the Hermite interpolant in Newton form.

Alternatively, we can match one more derivative f'' at $x = 1$ only:

x	$f[1]$	$f[2]$	$f[3]$	$f[4]$	$f[5]$
0	1	$\log 2$	$1 - \log 2$	$3\log 2 - 2$	$\log^2 2 - 5\log 2 + 3$
0	1	1	$2\log 2 - 1$	$\log^2 2 - 2\log 2 + 1$	
1	2	$2\log 2$	$\log^2 2$		
1	2	$2\log 2$			
1	2				

Note that $f[x_1, x_1, x_1] = f''(x_1)/2!$ contains a factor of 2! which is easy to forget about. The resulting interpolant is

$$p(x) = 1 + (\log 2)x + (1 - \log 2)x^2 + (3\log 2 - 2)x^2(x-1) + (\log^2 2 - 5\log 2 + 3)x^2(x-1)^2.$$

Error estimate Suppose p matches f and f' at $n+1$ points with degree $2n+1$. Inevitably the error must be

$$f(x) - p(x) = Cf^{(2n+2)}(\xi)\omega(x)^2$$

where the derivative ensures that polynomials of degree $2n+1$ are reproduced exactly (by uniqueness) and $\omega(x)^2$ ensures that p matches both f and f' at each x_j. Determine C by testing the formula on $f(x) = \omega(x)^2$ where the derivative is $(2n+2)!$: then $p(x) = 0$ so

$$f(x) - p(x) = \frac{1}{(2n+2)!} f^{(2n+2)}(\xi)\omega(x)^2.$$

A subtle advantage of Hermite interpolation is that for a given spacing $h = x_{j+1} - x_j$, the double roots of

$$\omega(x)^2 = (x - x_0)^2(x - x_1)^2 \cdots (x - x_n)^2$$

are twice as clustered as the single roots of the Lagrange equivalent of equal degree

$$\omega_{2n}(x) = (x - x_0)(x - x_1) \cdots (x - x_{2n+1}),$$

Thus the error bound will be smaller for Hermite with equal spacing.

Lagrange basis functions There are also Lagrange-type basis functions for Hermite interpolation. For example, we can build $(K+1)(n+1)$ polynomials $H_{jk}(x)$ of degree $(K+1)(n+1) - 1$, such that

$$H_{jk}^{(m)}(x_i) = \delta_{ij}\delta_{km}, \qquad 0 \le k \le K, \qquad 0 \le j \le n,$$

after which the Hermite interpolant is given by

$$p(x) = \sum_{k=0}^{K} \sum_{j=0}^{n} f^{(k)}(x_j) H_{jk}(x)$$

and satisfies

$$p^{(k)}(x_j) = f^{(k)}(x_j).$$

For $K = 1$ and $n = 1$ we need 4 cubic polynomials satisfying

$$H_{00}(x_0) = 1, H'_{00}(x_0) = 0, H_{00}(x_1) = 0, H'_{00}(x_1) = 0,$$

$$H_{10}(x_0) = 0, H'_{10}(x_0) = 0, H_{10}(x_1) = 1, H'_{10}(x_1) = 0,$$

$$H_{01}(x_0) = 0, H'_{01}(x_0) = 1, H_{01}(x_1) = 0, H'_{01}(x_1) = 0,$$

and

$$H_{11}(x_0) = 0, H'_{11}(x_0) = 0, H_{11}(x_1) = 0, H'_{11}(x_1) = 1.$$

These conditions are almost satisfied by the squares $L_j^2(x)$ of the usual Lagrange basis functions, since $L_j(x_i) = \delta_{ij}$ implies that $L_j^2(x_i) = \delta_{ij}$ as well. However, these polynomials (a) have degree only $2n$ rather than $2n+1$, and (b) have the wrong derivative values. Hence we should seek $H_{jk}(x)$ in the form $(a_{jk} + b_{jk}(x - x_j))L_j^2(x)$, after which the constants a_{jk} and b_{jk} must satisfy

$$a_{j0} = 1, \qquad b_{j0} = -2L'_j(x_j)$$

and

$$a_{j1} = 0, \qquad b_{j1} = 1.$$

Thus

$$H_{j0}(x) = (1 - 2L'_j(x_j))(x - x_j))L_j(x)^2$$

and

$$H_{j1}(x) = (x - x_j)L_j(x)^2.$$

Newton's formula can also be used to construct these basis functions, because they interpolate known values at the interpolation points.