

1. Interpolation in function and derivative values - Hermite interpolation

In addition to sampling of the function $f: \mathbb{R} \rightarrow \mathbb{R}$, information on the derivatives of f might also be available, as in the data set

$$\mathcal{D}' = \{(x_i, y_i = f(x_i), y'_i = f'(x_i)), i = 0, 1, \dots, n\}. \quad (1)$$

The extended data set can again be interpolated by a polynomial, this time of degree $2n + 1$ given in the monomial, Lagrange or Newton form.

Monomial form of interpolating polynomial. Using the monomial basis

$$\mathcal{M}_{2n+1}(t) = [1 \ t \ t^2 \ t^3 \ \dots \ t^{2n+1}],$$

the interpolating polynomial is

$$p(t) = \mathcal{M}_{2n+1}(t)\mathbf{a} = [1 \ t \ \dots \ t^{2n+1}] \begin{bmatrix} 0 \\ a_1 \\ \vdots \\ a_{2n+1} \end{bmatrix} = a_0 + a_1 t + \dots + a_{2n+1} t^{2n+1},$$

with derivative

$$p'(t) = a_1 + 2a_2 t + \dots + (2n+1)a_{2n+1} t^{2n}.$$

The above suggests constructing a basis set of monomials and their derivatives

$$\mathcal{M}'_{2n+1}(t) = \begin{bmatrix} 1 & t & t^2 & t^3 & \dots & t^{2n+1} \\ 0 & 1 & 2t & 3t^2 & \dots & (2n+1)t^{2n} \end{bmatrix},$$

to allow setting the function $p(x_i) = y_i$, and derivative conditions $p'(x_i) = y'_i$. The columns of $\mathcal{M}'_{2n+1}(t)$ are linearly independent since

$$\alpha \begin{bmatrix} t^j \\ jt^{j-1} \end{bmatrix} + \beta \begin{bmatrix} t^k \\ kt^{k-1} \end{bmatrix} = 0,$$

can only be satisfied for all t by $\alpha = \beta = 0$.

◦ Sampling at $\mathbf{x} \in \mathbb{R}^{(n+1)}$ gives $\mathbf{M} = \mathcal{M}'_{2n+1}(\mathbf{x}) \in \mathbb{R}^{(2n+2) \times (2n+2)}$, e.g., for $n = 2$, the matrix is

$$\mathbf{M} = \begin{pmatrix} 1 & x_0 & x_0^2 & x_0^3 & x_0^4 & x_0^5 \\ 1 & x_1 & x_1^2 & x_1^3 & x_1^4 & x_1^5 \\ 1 & x_2 & x_2^2 & x_2^3 & x_2^4 & x_2^5 \\ 0 & 1 & 2x_0 & 3x_0^2 & 4x_0^3 & 5x_0^4 \\ 0 & 1 & 2x_1 & 3x_1^2 & 4x_1^3 & 5x_1^4 \\ 0 & 1 & 2x_2 & 3x_2^2 & 4x_2^3 & 5x_2^4 \end{pmatrix},$$

is obtained.

For general n , \mathbf{M} is of full rank for distinct sample points with a determinant reminiscent of that of the Vandermonde matrix

$$\det(\mathbf{M}) = \prod_{0 \leq i < j \leq n} (x_i - x_j)^4.$$

The interpolation conditions lead to the linear system

$$\mathbf{M}\mathbf{a} = \begin{bmatrix} \mathbf{y} \\ \mathbf{y}' \end{bmatrix},$$

whose solution requires $\mathcal{O}([2(n+1)]^3/3)$ operations. An error formula is again obtained by repeated application of Rolle's theorem, i.e., for p interpolant of data set \mathcal{D}' , $\exists \xi_t \in (x_0, x_n)$ such that

$$f(t) - p(t) = \frac{f^{(2n+2)}(\xi_t)}{(2n+2)!} \prod_{j=0}^n (t - x_j)^2.$$

The above approach generalizes to higher-order derivatives, e.g., for

$$\mathcal{D}'' = \{(x_i, y_i = f(x_i), y'_i = f'(x_i), y''_i = f''(x_i)), i = 0, 1, \dots, n\}, \quad (2)$$

the basis set is

$$\mathcal{M}''_{3n+2}(t) = \begin{bmatrix} 1 & t & t^2 & t^3 & \dots & t^{3n+2} \\ 0 & 1 & 2t & 3t^2 & \dots & (3n+2)t^{3n+1} \\ 0 & 0 & 2 & 6t & \dots & (3n+2)(3n+1)t^{3n} \end{bmatrix},$$

with interpolant

$$p(t) = \mathcal{M}''_{3n+2}(t)\mathbf{a},$$

with $\mathbf{a} \in \mathbb{R}^{3(n+1)}$ determined by solving

$$\mathbf{M}\mathbf{a} = \begin{bmatrix} \mathbf{y} \\ \mathbf{y}' \\ \mathbf{y}'' \end{bmatrix}$$

with $\mathbf{M} = \mathcal{M}''_{3n+2}(\mathbf{x}) \in \mathbb{R}^{(3n+3) \times (3n+3)}$, and error formula

$$f(t) - p(t) = \frac{f^{(3n+3)}(\xi_t)}{(3n+3)!} \prod_{j=0}^n (t-x_j)^3.$$

Lagrange form of interpolating polynomial. As in the function value interpolation case, a basis set that evaluates to an identity matrix when sampled at $\mathbf{x} \in \mathbb{R}^{n+1}$ is obtained by LU -factorization of the sampled monomial matrix

$$\mathcal{M}'_{2n+1}(\mathbf{x}) = \mathbf{M} = \mathbf{L}\mathbf{U} = \mathbf{I}\mathbf{L}\mathbf{U} = \mathcal{L}'_{2n+1}(\mathbf{x})\mathbf{L}\mathbf{U},$$

that for arbitrary t leads to the basis set

$$\mathcal{L}'_{2n+1}(t) = \mathcal{M}'_{2n+1}(t)\mathbf{U}^{-1}\mathbf{L}^{-1} = \begin{bmatrix} a_0(t) & a_1(t) & \dots & a_n(t) & b_0(t) & b_1(t) & \dots & b_n(t) \\ a'_0(t) & a'_1(t) & \dots & a'_n(t) & b'_0(t) & b'_1(t) & \dots & b'_n(t) \end{bmatrix}.$$

The interpolating polynomial of data set $\mathcal{D}' = \{(x_i, y_i = f(x_i), y'_i = f'(x_i)), i = 0, 1, \dots, n\}$ is

$$p(t) = \sum_{i=0}^n y_i a_i(t) + \sum_{i=0}^n y'_i b_i(t),$$

where the basis functions can be expressed in terms of the Lagrange polynomials

$$\ell_i(t) = \prod_{j=0}^{n'} \frac{t-x_j}{x_i-x_j},$$

as

$$a_i(t) = [1 - 2(t-x_i)\ell'_i(x_i)]\ell_i^2(t), \quad b_i(t) = (t-x_i)\ell_i^2(t),$$

and have the properties

$$a_i(x_j) = \delta_{ij}, \quad a'_i(x_j) = 0, \quad b_i(x_j) = 0, \quad b'_i(x_j) = \delta_{ij}.$$

- As, an example, consider the LU -factorization of matrix $\mathbf{M} = \mathcal{M}'_{2n+1}(\mathbf{x})$ for $n = 1$

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & \frac{1}{x_0-x_1} & 1 & 0 \\ 0 & \frac{1}{x_0-x_1} & -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & \frac{1}{x_1-x_0} & 1 & 0 \\ 0 & \frac{1}{x_1-x_0} & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & x_0 & x_0^2 & x_0^3 \\ 0 & x_1-x_0 & x_1^2-x_0^2 & x_1^3-x_0^3 \\ 0 & 0 & x_0-x_1 & 2x_0^2-x_1x_0-x_1^2 \\ 0 & 0 & 0 & (x_0-x_1)^2 \end{pmatrix}.$$

- The factor inverses are

$$\mathbf{L}^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ \frac{1}{x_1-x_0} & \frac{1}{x_0-x_1} & 1 & 0 \\ \frac{2}{x_1-x_0} & \frac{2}{x_0-x_1} & 1 & 1 \end{pmatrix}, \quad \mathbf{U}^{-1} = \begin{pmatrix} 1 & \frac{x_0}{x_0-x_1} & \frac{x_0x_1}{x_0-x_1} & -\frac{x_0^2x_1}{(x_0-x_1)^2} \\ 0 & \frac{1}{x_1-x_0} & \frac{x_0+x_1}{x_0-x_1} & \frac{x_0(x_0+2x_1)}{(x_0-x_1)^2} \\ 0 & 0 & \frac{1}{x_0-x_1} & \frac{2x_0+x_1}{(x_0-x_1)^2} \\ 0 & 0 & 0 & \frac{1}{(x_0-x_1)^2} \end{pmatrix}$$

- The functions that result

$$\left\{ \left[1 - 2(t-x_0) \frac{1}{x_0-x_1} \right] \left(\frac{t-x_1}{x_0-x_1} \right)^2, \left[1 - 2(t-x_1) \frac{1}{x_1-x_0} \right] \left(\frac{t-x_0}{x_1-x_0} \right)^2, (t-x_0) \left(\frac{t-x_1}{x_0-x_1} \right)^2, (t-x_1) \left(\frac{t-x_0}{x_1-x_0} \right)^2 \right\},$$

are indeed expressed in terms of $\ell_i(t)$ as

$$\{ [1 - 2(t-x_0) \ell'_0(x_0)] \ell_0^2(t), [1 - 2(t-x_1) \ell'_1(x_1)] \ell_1^2(t), (t-x_0) \ell_0^2(t), (t-x_1) \ell_1^2(t) \}.$$

The procedure can be extended to derivatives of arbitrary order, e.g., the data set \mathcal{D}'' is interpolated by

$$p(t) = \sum_{i=0}^n y_i a_i(t) + \sum_{i=0}^n y'_i b_i(t) + \sum_{i=0}^n y''_i c_i(t),$$

where the Lagrange basis polynomials are given as

$$\mathcal{L}_{3n+2}''(t) = \mathcal{M}_{3n+2}''(t) \mathbf{U}^{-1} \mathbf{L}^{-1} = \begin{bmatrix} a_0(t) & \dots & a_n(t) & b_0(t) & \dots & b_n(t) & c_0(t) & \dots & c_n(t) \\ a'_0(t) & \dots & a'_n(t) & b'_0(t) & \dots & b'_n(t) & c'_0(t) & \dots & c'_n(t) \\ a''_0(t) & \dots & a''_n(t) & b''_0(t) & \dots & b''_n(t) & c''_0(t) & \dots & c''_n(t) \end{bmatrix}.$$

Newton form of interpolating polynomial. As before, inverting only one factor of the $\mathcal{M}'_{2n+1}(t) = \mathcal{L}'_{2n+1}(t) \mathbf{L} \mathbf{U}$ mapping yields a triangular basis set $\mathcal{S}'(t) = [s_0(t) \ s_1(t) \ s_2(t) \ \dots]$

$$\mathcal{M}'_{2n+1}(t) \mathbf{U}^{-1} = \mathcal{S}'_{2n+1}(t).$$

- The first six basis polynomials obtained for $n=2$ are

$$\left\{ 1, \frac{t-x_0}{x_1-x_0}, \frac{(t-x_0)(t-x_1)}{(x_2-x_0)(x_2-x_1)}, \frac{(t-x_0)(t-x_1)(t-x_2)}{(x_2-x_0)(x_1-x_0)}, \frac{(t-x_0)^2(t-x_1)(t-x_2)}{(x_1-x_0)^2(x_1-x_2)}, \frac{(t-x_0)^2(t-x_1)^2(t-x_2)}{(x_2-x_0)^2(x_2-x_1)^2} \right\}.$$

- A closer link to divided difference and differential calculus is obtained by permuting rows of \mathbf{M} , e.g., for $n=2$

$$\mathbf{PM} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & x_0 & x_0^2 & x_0^3 & x_0^4 & x_0^5 \\ 1 & x_1 & x_1^2 & x_1^3 & x_1^4 & x_1^5 \\ 1 & x_2 & x_2^2 & x_2^3 & x_2^4 & x_2^5 \\ 0 & 1 & 2x_0 & 3x_0^2 & 4x_0^3 & 5x_0^4 \\ 0 & 1 & 2x_1 & 3x_1^2 & 4x_1^3 & 5x_1^4 \\ 0 & 1 & 2x_2 & 3x_2^2 & 4x_2^3 & 5x_2^4 \end{pmatrix} = \begin{pmatrix} 1 & x_0 & x_0^2 & x_0^3 & x_0^4 & x_0^5 \\ 0 & 1 & 2x_0 & 3x_0^2 & 4x_0^3 & 5x_0^4 \\ 1 & x_1 & x_1^2 & x_1^3 & x_1^4 & x_1^5 \\ 0 & 1 & 2x_1 & 3x_1^2 & 4x_1^3 & 5x_1^4 \\ 1 & x_2 & x_2^2 & x_2^3 & x_2^4 & x_2^5 \\ 0 & 1 & 2x_2 & 3x_2^2 & 4x_2^3 & 5x_2^4 \end{pmatrix}.$$

The first six basis polynomials thus obtained are

$$\left\{ 1, t-x_0, \frac{(t-x_0)^2}{(x_1-x_0)^2}, \frac{(t-x_0)^2(t-x_1)}{(x_1-x_0)^2}, \frac{(t-x_0)^2(t-x_1)^2}{(x_2-x_0)^2(x_2-x_1)^2}, \frac{(t-x_0)^2(t-x_1)^2(t-x_2)}{(x_2-x_0)^2(x_2-x_1)^2} \right\}.$$

and upon rescaling generalize to the basis set

$$\mathcal{N}'_{2n+1}(t) = [n_0(t) \ n_1(t) \ \dots \ n_{2n+1}(t)],$$

with

$$n_{2k}(t) = \prod_{j=0}^{k-1} (t-x_j)^2, n_{2k+1}(t) = (t-x_k) n_{2k}(t), k=0, 1, \dots, n$$

known as the Newton basis set with repetitions.

The interpolating polynomial in Newton divided difference form is

$$p(t) = [y_0] + [y_0, y_0](t-x_0) + [y_1, y_0, y_0](t-x_0)^2 + \dots + [y_n, y_n, \dots, y_0, y_0](t-x_0)^2 \dots (t-x_{n-1})^2 (t-x_n).$$

Divided difference with repeated values are replaced by their, limits, i.e., the derivatives

$$[y_k, y_k] = \lim_{x_{k-1} \rightarrow x_k} \frac{y_k - y_{k-1}}{x_k - x_{k-1}} = y'_k.$$

The forward substitution can again be organized in a table.

i	x_i	$[y_i]$	$[y_i, y_{i-1}]$	$[y_i, y_{i-1}, y_{i-2}]$	
0	x_0	y_0	-	-	
0	x_0	y_0	y_0'		
1	x_1	y_1	$\frac{y_1 - y_0}{x_1 - x_0}$	$\frac{1}{x_1 - x_0} \left(\frac{y_1 - y_0}{x_1 - x_0} - y_0' \right)$	
1	x_1	y_1	y_1'	$\frac{1}{x_1 - x_0} \left(y_1' - \frac{y_1 - y_0}{x_1 - x_0} \right)$	
2	x_2	y_2	$\frac{y_2 - y_1}{x_2 - x_1}$	$\frac{1}{x_2 - x_1} \left(\frac{y_2 - y_1}{x_2 - x_1} - y_1' \right)$	\dots
2	x_2	y_2	y_2'		
\vdots	\vdots	\vdots	\vdots		
n	x_n	y_n	y_n'	$\frac{1}{x_n - x_{n-1}} \left(y_n' - \frac{y_n - y_{n-1}}{x_n - x_{n-1}} \right)$	$\dots \frac{[y_n, \dots, y_1] - [y_{n-1}, \dots, y_0]}{x_n - x_0}$

Table 1. Table of repeated divided differences. The Newton basis coefficients are the diagonal terms.

Interpolation of data containing higher derivatives, or differing orders of derivative information at each node are possible. For multiple repeated values arising in the limit $x_{i+k} \rightarrow x_i$ of sample points $x_i \leq x_{i+1} \leq \dots \leq x_{i+k}$ the divided difference is determined by

$$[y_{i+k}, y_{i+k-1}, \dots, y_i] = \begin{cases} \frac{[y_{i+k}, y_{i+k-1}, \dots, y_{i+1}] - [y_{i+k-1}, y_{i+k-1}, \dots, y_i]}{x_{i+k} - x_i} & x_i < x_{i+k} \\ \frac{y_i^{(k)}}{k!} & x_i = x_{i+k} \end{cases} .$$