Interpolation

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The interpolation used in TabProps requires continuous derivatives (up to some specified order) and uses Lagrange polynomials to accomplish this. These can be fast and efficient for both uniform and nonuniform tabulated data.

1 One-Dimensional Interpolation

Lagrange polynomials provide arbitrary-order interpolants that are also smooth. For an interpolant of order n, these provide interpolants that are smooth for derivatives up to order $n-1$.

$$f(x) = \sum_{k=0}^{n} y_k L_k(x) \tag{1}$$

with

$$L_k(x) = \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{x-x_i}{x_k-x_i}. \tag{2}$$

For example, second-order interpolants $(n=2)$ would be given by (2) as

$$\begin{aligned} L_0(x) &= \frac{x-x_1}{x_0-x_1}\frac{x-x_2}{x_0-x_2}, \\ L_1(x) &= \frac{x-x_0}{x_1-x_0}\frac{x-x_2}{x_1-x_2}, \\ L_2(x) &= \frac{x-x_0}{x_2-x_0}\frac{x-x_1}{x_2-x_1} \end{aligned}$$

and

$$f(x) = y_0 L_0(x) + y_1 L_1(x) + y_2 L_2(x)$$

where the points 0, 1 and 2 correspond to the data points closest to the given value of x.

This can be done on uniform or nonuniform grids.

1.1 Differentiation

The Lagrange polynomial basis functions given by (2) may be differentiated to obtain

$$L_k'(x) = \left[\sum_{\substack{i=0\\ i\neq k}}^{n} \frac{1}{x_k-x_i} \prod_{\substack{j=0\\ j\neq i,k}}^{n} \frac{x-x_j}{x_k-x_j} \right] \tag{3}$$

so that we have

$$f'(x) = \sum_{k=0}^{n} y_k L'_k(x). \tag{4}$$

For example, second-order interpolants would have linear derivatives with (3) giving

$$\begin{aligned}
L'_0(x) &= \frac{1}{x_0 - x_1}\frac{x - x_2}{x_0 - x_2} + \frac{1}{x_0 - x_2}\frac{x - x_1}{x_0 - x_1}, \\
L'_1(x) &= \frac{1}{x_1 - x_0}\frac{x - x_2}{x_1 - x_2} + \frac{1}{x_1 - x_2}\frac{x - x_0}{x_1 - x_0}, \\
L'_2(x) &= \frac{1}{x_2 - x_0}\frac{x - x_1}{x_2 - x_1} + \frac{1}{x_2 - x_1}\frac{x - x_0}{x_2 - x_0}.
\end{aligned}$$

Similarly, for second-order derivatives, (3) can be differentiatied to obtain

$$L''_k(x) = \sum_{\substack{i=0 \\ i\neq k}}^{n} \frac{1}{x_k - x_i} \sum_{\substack{j=0 \\ j\neq i,k}}^{n} \frac{1}{x_k - x_j} \prod_{\substack{\ell=0 \\ \ell\neq i,j,k}}^{n} \frac{x - x_\ell}{x_k - x_\ell}. \tag{5}$$

so that we find

$$f''(x) = \sum_{k=0}^{n} y_k L''_k(x). \tag{6}$$

For example, second-order interpolants would have constant second derivatives with (5) giving

$$\begin{aligned}
L''_0(x) &= \frac{1}{x_0 - x_1}\frac{1}{x_0 - x_2} + \frac{1}{x_0 - x_2}\frac{1}{x_0 - x_1}, \\
L''_1(x) &= \frac{1}{x_1 - x_0}\frac{1}{x_1 - x_2} + \frac{1}{x_1 - x_2}\frac{1}{x_1 - x_0}, \\
L''_2(x) &= \frac{1}{x_2 - x_0}\frac{1}{x_2 - x_1} + \frac{1}{x_2 - x_1}\frac{1}{x_2 - x_0}.
\end{aligned}$$

2 Two-Dimensional Interpolation

The Lagrange interpolation formula in 2D is

$$f(x, y) = \sum_{k_x=0}^{n} \sum_{k_y=0}^{n} f(x_{k_x}, y_{k_y}) L_{k_x}(x) L_{k_y}(y) \tag{7}$$

with

$$\begin{aligned}
L_{k_X}(x) &= \prod_{\substack{i=0 \\ i\neq k}}^{n} \frac{x - x_i}{x_{k_x} - x_i}, &(8) \\
L_{k_y}(y) &= \prod_{\substack{i=0 \\ i\neq k}}^{n} \frac{y - y_i}{y_{k_y} - y_i} &(9)
\end{aligned}$$

2.1 Differentiation

Equations (8) and (9) may be differentiated to obtain

$$
\begin{aligned}
L_k'(x) &= \sum_{\substack{i=0\\ i\neq k}}^{n} \frac{1}{x_{k_x}-x_i} \prod_{\substack{j=0\\ j\neq i,k}}^{n} \frac{x-x_j}{x_{k_x}-x_j}, & (10)\\
L_k'(y) &= \sum_{\substack{i=0\\ i\neq k}}^{n} \frac{1}{y_{k_y}-y_i} \prod_{\substack{j=0\\ j\neq i,k}}^{n} \frac{y-y_j}{y_{k_y}-y_j}. & (11)
\end{aligned}
$$

with

$$
\begin{aligned}
\frac{\partial f}{\partial x} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n} f(x_{k_x},y_{k_y})L_{k_x}'(x)L_{k_y}(y). & (12)\\
\frac{\partial f}{\partial y} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n} f(x_{k_x},y_{k_y})L_{k_x}(x)L_{k_y}'(y). & (13)
\end{aligned}
$$

Similarly, second derivatives are obtained by differentiating (12) and (13) to obtain

$$
\begin{aligned}
\frac{\partial^2 f}{\partial x^2} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n} f(x_{k_x},y_{k_y})L_{k_x}''(x)L_{k_y}(y), & (14)\\
\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n} f(x_{k_x},y_{k_y})L_{k_x}'(x)L_{k_y}'(y), & (15)\\
\frac{\partial^2 f}{\partial y^2} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n} f(x_{k_x},y_{k_y})L_{k_x}(x)L_{k_y}''(y) & (16)
\end{aligned}
$$

with $L_{k_x}''(x)$ and $L_{k_{uy}}''(y)$ given by (5).

3 Three-Dimensional Interpolation

The Lagrange interpolation formula in 3D is

$$
f(x,y) = \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x},y_{k_y},z_{k_z})L_{k_x}(x)L_{k_y}(y)L_{k_z}(z)
$$

with

$$
\begin{aligned}
L_k(x) &= \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{x-x_i}{x_k-x_i},\\
L_k(y) &= \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{y-y_i}{y_k-y_i},\\
L_k(z) &= \prod_{\substack{i=0\\ i\neq k}}^{n} \frac{z-z_i}{z_k-z_i}.
\end{aligned}
$$

The first and second derivative operations are straightforward extensions of those for 1D and 2D. Namely, for first derivatives,

$$
\begin{aligned}
\frac{\partial f}{\partial x} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L'_{k_x}(x) L_{k_y}(y) L_{k_z}(z), \\
\frac{\partial f}{\partial y} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L_{k_x}(x) L'_{k_y}(y) L_{k_z}(z) \\
\frac{\partial f}{\partial z} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L_{k_x}(x) L_{k_y}(y) L'_{k_z}(z)
\end{aligned}
$$

with L' given by (3). Similarly, for second derivatives

$$
\begin{aligned}
\frac{\partial^2 f}{\partial x^2} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L''_{k_x}(x) L_{k_y}(y) L_{k_z}(z), && (17) \\
\frac{\partial^2 f}{\partial y^2} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L_{k_x}(x) L''_{k_y}(y) L_{k_z}(z), && (18) \\
\frac{\partial^2 f}{\partial z^2} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L_{k_x}(x) L_{k_y}(y) L''_{k_z}(z), && (19) \\
\frac{\partial^2 f}{\partial x \partial y} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L'_{k_x}(x) L'_{k_y}(y) L_{k_z}(z), && (20) \\
\frac{\partial^2 f}{\partial x \partial z} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L'_{k_x}(x) L_{k_y}(y) L'_{k_z}(z), && (21) \\
\frac{\partial^2 f}{\partial y \partial z} &= \sum_{k_x=0}^{n}\sum_{k_y=0}^{n}\sum_{k_z=0}^{n} f(x_{k_x}, y_{k_y}, z_{k_z}) L_{k_x}(x) L'_{k_y}(y) L'_{k_z}(z), && (22)
\end{aligned}
$$

with L' and L'' given by (3) and (5), respectively.