Cubic Interpolation & Derivatives in d Dimensions

Oliver K. Ernst
UCSD Physics

September 19, 2018

Contents

1 In one dimension

1.1 Interpolation

Consider a 1D grid of points of length n, with abscissas $(s_0, \dots, s_{n-1})$.

Let values be defined on each point, given by $(t_0, \dots, t_{n-1})$.

Given a point $\tilde{x}$ that falls between two abscissas s_i, s_{i+1}, define the surrounding values: $p_0 = t_{i-1}, p_1 = t_i, p_2 = t_{i+1}, p_3 = t_{i+2}$.

Let x be the **fraction** that $\tilde{x}$ is between the two neighboring points, i.e. $x = (\tilde{x} - s_i)/(s_{i+1} - s_i)$.

The cubic interpolation formula is:

$$f(x; p_0, p_1, p_2, p_3) = \left(-\frac{1}{2}p_0 + \frac{3}{2}p_1 - \frac{3}{2}p_2 + \frac{1}{2}p_3 \right) x^3 + \left(p_0 - \frac{5}{2}p_1 + 2p_2 - \frac{1}{2}p_3 \right) x^2 + \left(-\frac{1}{2}p_0 + \frac{1}{2}p_2 \right) x + p_1 \tag{1}$$

In case the point falls near the boundary, then either the point p_0 or p_3 does not exist, and needs to be approximated. The best approximation is a linear one:

$$\begin{aligned} & p_0 \approx 2p_1 - p_2 \\ \text{or} \quad & p_3 \approx 2p_2 - p_1 \end{aligned} \tag{2}$$

1.2 The derivative with respect to a point value

The derivatives with respect to a grid point values are:

$$
\begin{aligned}
\frac{df}{dp_0} &= -\frac{1}{2}x^3 + x^2 - \frac{1}{2}x \\
\frac{df}{dp_1} &= \frac{3}{2}x^3 - \frac{5}{2}x^2 + 1 \\
\frac{df}{dp_2} &= -\frac{3}{2}x^3 + 2x^2 + \frac{1}{2}x \\
\frac{df}{dp_3} &= \frac{1}{2}x^3 - \frac{1}{2}x^2
\end{aligned}
\tag{3}
$$

If the point falls near the boundary, and we approximate $p_0 \approx 2p_1 - p_2$, we have instead:

$$
\begin{aligned}
\frac{df}{dp_1} &= \frac{\partial f}{\partial p_1} + \frac{\partial f}{\partial p_0}\frac{\partial p_0}{\partial p_1} = \frac{1}{2}x^3 - \frac{1}{2}x^2 - x + 1 \\
\frac{df}{dp_2} &= \frac{\partial f}{\partial p_2} + \frac{\partial f}{\partial p_0}\frac{\partial p_0}{\partial p_2} = -x^3 + x^2 + x \\
\frac{df}{dp_3} &= \frac{1}{2}x^3 - \frac{1}{2}x^2
\end{aligned}
\tag{4}
$$

If it falls near the other boundary and we approximate $p_3 \approx 2p_2 - p_1$, we have:

$$
\begin{aligned}
\frac{df}{dp_0} &= -\frac{1}{2}x^3 + x^2 - \frac{1}{2}x \\
\frac{df}{dp_1} &= \frac{\partial f}{\partial p_1} + \frac{\partial f}{\partial p_3}\frac{\partial p_3}{\partial p_1} = x^3 - 2x^2 + 1 \\
\frac{df}{dp_2} &= \frac{\partial f}{\partial p_2} + \frac{\partial f}{\partial p_3}\frac{\partial p_3}{\partial p_2} = -\frac{1}{2}x^3 + x^2 + \frac{1}{2}x
\end{aligned}
\tag{5}
$$

1.3 The derivative with respect to x

The derivative with respect to the point $\tilde{x}$ is:

$$
\begin{aligned}
\frac{\partial f}{\partial x} &= 3\left(-\frac{1}{2}p_0 + \frac{3}{2}p_1 - \frac{3}{2}p_2 + \frac{1}{2}p_3\right)x^2 + 2\left(p_0 - \frac{5}{2}p_1 + 2p_2 - \frac{1}{2}p_3\right)x - \frac{1}{2}p_0 + \frac{1}{2}p_2 \\
\frac{\partial f}{\partial \tilde{x}} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial \tilde{x}} = \frac{\partial f}{\partial x}\left(s_{i+1} - s_i\right)^{-1}
\end{aligned}
\tag{6}
$$

If the point falls near the boundary, the result is unchanged.

2 In d-dimensions

2.1 Interpolation

In d dimensions, let the grid abscissas in each dimension be $(s^d_0, \ldots, s^d_{n_d-1})$ of length n_d.

The grid points are then:

$$
\boldsymbol{s}^{[d]:\langle j_1,\ldots,j_d\rangle} = \left(s^1_{j_1}, \ldots, s^d_{j_d}\right)
\tag{7}
$$

Here, we use the notation $\boldsymbol{s}^{[d]:\langle j_1,\ldots,j_d\rangle}$ that there is one of such vector (of dimension d) for every set of d indexes $\langle j_1, \ldots, j_d\rangle$.

Let the values associated with each grid point be:

$$t^{[d]:\langle j_1,\ldots,j_d\rangle} \tag{8}$$

To further reduce the burden of indexing, define:

$$[d]:\langle 1:d\rangle = [d]:\langle j_1,\ldots,j_d\rangle \tag{9}$$

when specific indexes are not needed, then the abscissas and associated points are:

$$\boldsymbol{s}^{[d]:\langle 1:d\rangle}$$
$$t^{[d]:\langle 1:d\rangle}$$

Given a point $\tilde{\boldsymbol{x}} = (\tilde{x}^1,\ldots,\tilde{x}^d)$ of dimension d that falls between grid points $s^d_{i_d}, s^d_{i_{d+1}}$ in each dimension, define the values $p^{[d]:\langle 1:d\rangle}$:

$$\begin{aligned}
p^{[d]:\langle 0,\ldots,0,0\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1}-1,i_d-1\rangle}\\
p^{[d]:\langle 0,\ldots,0,1\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1}-1,i_d\rangle}\\
p^{[d]:\langle 0,\ldots,0,2\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1}-1,i_d+1\rangle}\\
p^{[d]:\langle 0,\ldots,0,3\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1}-1,i_d+2\rangle}\\
p^{[d]:\langle 0,\ldots,1,0\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1},i_d-1\rangle}\\
p^{[d]:\langle 0,\ldots,2,0\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1}+1,i_d-1\rangle}\\
p^{[d]:\langle 0,\ldots,3,0\rangle} &= t^{[d]:\langle i_1-1,\ldots,i_{d-1}+2,i_d-1\rangle}
\end{aligned}$$

etc., or more generally

$$p^{[d]:\langle j_1,\ldots,j_d\rangle} = t^{[d]:\langle i_1-1+j_1,\ldots,i_d-1+j_d\rangle}$$

where $j = 0,1,2,3$.

There are 4^d of such points $p^{[d]:\langle 1:d\rangle}$ in total.

Let $\boldsymbol{x}$ be the fraction with components:

$$x_\delta = (\tilde{x}^\delta - s^\delta_{i_\delta})/(s^\delta_{i_\delta+1} - s^\delta_{i_\delta}) \tag{10}$$

for $\delta = 1,\ldots,d$.

The cubic interpolation now proceeds iteratively - define points $p^{[d-1]:\langle 2:d\rangle}$:

$$p^{[d-1]:\langle j_2,\ldots,j_d\rangle} = f\left(x_1; p^{[d]:\langle 0,j_2,\ldots,j_d\rangle}, p^{[d]:\langle 1,j_2,\ldots,j_d\rangle}, p^{[d]:\langle 2,j_2,\ldots,j_d\rangle}, p^{[d]:\langle 3,j_2,\ldots,j_d\rangle}\right) \tag{11}$$

(notice the indexes appearing on the left), for all $i = 0,1,2,3$, or equivalently and more compactly:

$$p^{[d-1]:\langle 2:d\rangle} = f\left(x_1; p^{[d]:\langle 0,2:d\rangle}, p^{[d]:\langle 1,2:d\rangle}, p^{[d]:\langle 2,2:d\rangle}, p^{[d]:\langle 3,2:d\rangle}\right) \tag{12}$$

There are 4^{d-1} of such points $p^{[d-1]:\langle 2:d\rangle}$.

In general, the recursion relation to go from dimension δ to $\delta-1$ is:

$$p^{[\delta-1]:\langle d-\delta+2:d\rangle} = f\left(x_{d-\delta+1}; p^{[\delta]:\langle 0,d-\delta+2:d\rangle}, p^{[\delta]:\langle 1,d-\delta+2:d\rangle}, p^{[\delta]:\langle 2,d-\delta+2:d\rangle}, p^{[\delta]:\langle 3,d-\delta+2:d\rangle}\right) \tag{13}$$

We can continue this way until we reach the the last dimension $d = 0$, and are out of indexes on the left:

$$p^{[0]} = f\left(x_d; p^{[1]:\langle 0\rangle}, p^{[1]:\langle 1\rangle}, p^{[1]:\langle 2\rangle}, p^{[1]:\langle 3\rangle}\right) \tag{14}$$

is the desired interpolated value we seek.

2.1.1 Pseudocode

1. function **iterate**(δ, d, $\boldsymbol{x}$, $(j_2, \ldots, j_d)$, $p^{[d]:\langle 1:d\rangle}$):
   // With argument δ, this tries to return $p^{[\delta-1]:\langle d-\delta+2:d\rangle}$ = left side of (13)
   (a) if $\delta == d$: // Arrived at (12) which we can do with the points given
      i. return $f\left(x_1, p^{[d]:\langle 0,2:d\rangle}, p^{[d]:\langle 1,2:d\rangle}, p^{[d]:\langle 2,2:d\rangle}, p^{[d]:\langle 3,2:d\rangle}\right)$ // $= p^{[d-1]}$
   (b) else: // Go a level higher using (13)
      i. $p^{[\delta]:\langle 0,d-\delta+2:d\rangle}$ = **iterate**($\delta+1$, d, $\boldsymbol{x}$, $(j_2, \ldots, j_{d-\delta+1} = 0, \ldots, j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      ii. $p^{[\delta]:\langle 1,d-\delta+2:d\rangle}$ = **iterate**($\delta+1$, d, $\boldsymbol{x}$, $(j_2, \ldots, j_{d-\delta+1} = 1, \ldots, j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      iii. $p^{[\delta]:\langle 2,d-\delta+2:d\rangle}$ = **iterate**($\delta+1$, d, $\boldsymbol{x}$, $(j_2, \ldots, j_{d-\delta+1} = 2, \ldots, j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      iv. $p^{[\delta]:\langle 3,d-\delta+2:d\rangle}$ = **iterate**($\delta+1$, d, $\boldsymbol{x}$, $(j_2, \ldots, j_{d-\delta+1} = 3, \ldots, j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      v. return $f\left(x_{d-\delta+1}; p^{[\delta]:\langle 0,d-\delta+2:d\rangle}, p^{[\delta]:\langle 1,d-\delta+2:d\rangle}, p^{[\delta]:\langle 2,d-\delta+2:d\rangle}, p^{[\delta]:\langle 3,d-\delta+2:d\rangle}\right)$ // $= p^{[\delta-1]}$
2. To start: **iterate**(1,d,$\boldsymbol{x}$,$(j_2, \ldots, j_d)$,$p^{[d]:\langle 1:d\rangle}$)

2.2 The derivative with respect to a point value

What is the derivative with respect to a point value?

Let the point to differentiate with respect to be:

$$p^{[d]:\langle k_1,\ldots,k_d\rangle} \tag{15}$$

Then we seek:

$$\frac{\partial p^{[0]}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} \tag{16}$$

Using (14) and the chain rule:

$$\frac{\partial p^{[0]}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} = \sum_{j_d=0}^{3} \frac{\partial f\left(x_d; p^{[1]:\langle 0\rangle}, p^{[1]:\langle 1\rangle}, p^{[1]:\langle 2\rangle}, p^{[1]:\langle 3\rangle}\right)}{\partial p^{[1]:\langle j_d\rangle}} \frac{\partial p^{[1]:\langle j_d\rangle}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} \tag{17}$$

The first term can be evaluated using (3). We immediately notice an important property: the interpolation is linear in the point values, such that the first term does not depend on them. This greatly reduces the complexity - we use the notation from (3):

$$\frac{\partial f(x_d)}{\partial p_{j_d}} \tag{18}$$

to denote the derivative, giving:

$$\frac{\partial p^{[0]}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} = \sum_{j_d=0}^{3} \frac{\partial f(x_d)}{\partial p_{j_d}} \frac{\partial p^{[1]:\langle j_d\rangle}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} \tag{19}$$

The numerator of the second term is one dimension higher than the left hand side; this then is another recursion relation. Going another level gives:

$$\frac{\partial p^{[0]}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} = \sum_{j_{d-1}=0}^{3} \sum_{j_d=0}^{3} \frac{\partial f(x_d)}{\partial p_{j_d}} \frac{\partial f(x_{d-1})}{\partial p_{j_{d-1}}} \frac{\partial p^{[2]:\langle j_{d-1},j_d\rangle}}{\partial p^{[d]:\langle k_1,\ldots,k_d\rangle}} \tag{20}$$

After d such recursions:

$$
\begin{aligned}
\frac{\partial p^{[0]}}{\partial p^{[d]:\langle k_1,\dots,k_d\rangle}} &= \sum_{j_1,\dots,j_d} \left(\prod_{\alpha=1}^{d} \frac{\partial f(x_{d-\alpha+1})}{\partial p_{j_{d-\alpha+1}}} \right) \left(\frac{\partial p^{[d]:\langle j_1,\dots,j_d\rangle}}{\partial p^{[d]:\langle k_1,\dots,k_d\rangle}} \right) \\
&= \sum_{j_1,\dots,j_d} \left(\prod_{\alpha=1}^{d} \frac{\partial f(x_{d-\alpha+1})}{\partial p_{j_{d-\alpha+1}}} \right) \left(\prod_{\beta=1}^{d} \delta_{j_\beta,k_\beta} \right) \\
&= \prod_{\alpha=1}^{d} \frac{\partial f(x_{d-\alpha+1})}{\partial p_{k_{d-\alpha+1}}}
\end{aligned} \tag{21}
$$

This is in fact quite easy to evaluate, and does not require recursion!

2.3 The derivative with respect to x

We seek the derivative with respect to the k-th component x_k of $\boldsymbol{x}$:

$$
\frac{\partial p^{[0]}}{\partial x_k} \tag{22}
$$

Using (14):

$$
\frac{\partial p^{[0]}}{\partial x_k} = \frac{\partial f\left(x_d; p^{[1]:\langle 0\rangle}, p^{[1]:\langle 1\rangle}, p^{[1]:\langle 2\rangle}, p^{[1]:\langle 3\rangle}\right)}{\partial x_k} \tag{23}
$$

If $k = d$, the problem is trivially the 1D case given by (6).

If $k < d$, then using the chain rule:

$$
\frac{\partial p^{[0]}}{\partial x_k} = \sum_{j_d=0}^{3} \frac{\partial f\left(x_d; p^{[1]:\langle 0\rangle}, p^{[1]:\langle 1\rangle}, p^{[1]:\langle 2\rangle}, p^{[1]:\langle 3\rangle}\right)}{\partial p^{[1]:\langle j_d\rangle}} \frac{\partial p^{[1]:\langle j_d\rangle}}{\partial x_k} \tag{24}
$$

We again notice as before that the first term can be evaluated using (3) and does not depend on the point values p. Using the notation from (3):

$$
\frac{\partial f(x_d)}{\partial p_{j_d}} \tag{25}
$$

gives:

$$
\frac{\partial p^{[0]}}{\partial x_k} = \sum_{j_d=0}^{3} \frac{\partial f(x_d)}{\partial p_{j_d}} \frac{\partial p^{[1]:\langle j_d\rangle}}{\partial x_k} \tag{26}
$$

This again defines a recursion relation - more generally, differentiating (13) gives:

$$
\frac{\partial p^{[\delta-1]:\langle d-\delta+2:d\rangle}}{\partial x_k} = \sum_{j_{d-\delta+1}=0}^{3} \frac{\partial f(x_{d-\delta+1})}{\partial p_{j_{d-\delta+1}}} \frac{\partial p^{[\delta]:\langle d-\delta+1:d\rangle}}{\partial x_k} \tag{27}
$$

after $d-k$ such recursions:

$$
\frac{\partial p^{[0]}}{\partial x_k} = \sum_{j_{k+1},\dots,j_d} \left(\prod_{\alpha=1}^{d-k} \frac{\partial f(x_{d-\alpha+1})}{\partial p_{j_{d-\alpha+1}}} \right) \frac{\partial p^{[d-k]:\langle j_{k+1}:j_d\rangle}}{\partial x_k} \tag{28}
$$

which can be evaluated by noting that:

$$
\frac{\partial p^{[d-k]:\langle j_{k+1}:j_d\rangle}}{\partial x_k} = \frac{\partial f\left(x_k; p^{[d-k+1]:\langle 0,j_{k+1}:j_d\rangle}, p^{[d-k+1]:\langle 1,j_{k+1}:j_d\rangle}, p^{[d-k+1]:\langle 2,j_{k+1}:j_d\rangle}, p^{[d-k+1]:\langle 3,j_{k+1}:j_d\rangle}\right)}{\partial x_k} \tag{29}
$$

This can be evaluated using the 1D result (6) for the second term; unfortunately, this requires $k-1$ levels of recursion to determine the $p^{[d-k+1]}$.

Also: do not forget that:

$$\frac{\partial p^{[0]}}{\partial \tilde{x}_k} = \frac{\partial p^{[0]}}{\partial x_k}\frac{\partial x_k}{\partial \tilde{x}_k} = \frac{\partial p^{[0]}}{\partial x_k}\left(s^k_{i_k+1} - s^k_{i_k}\right)^{-1} \tag{30}$$

since $\boldsymbol{x}$ refers to a fraction between $0, 1$.

2.3.1 Pseudocode

1. function **iterate_deriv**(δ,k,d,$\boldsymbol{x}$,$(j_{k+1},\dots,j_d)$, $p^{[d]:\langle 1:d\rangle}$):
   // With arg δ, this evaluates $\partial p^{[\delta-1]:\langle d-\delta+2:d\rangle}/\partial x_k$ = the left hand of (27)

   (a) if $\delta == d-k+1$: // Evaluate the derivative on the right of (29)
      i. $p^{[d-k+1]:\langle 0,j_{k+1}:j_d\rangle}$ = **iterate**($d-k+2$, d, $\boldsymbol{x}$, $(j_k=0,j_{k+1},\dots,j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      // Recall that **iterate**($\delta,\dots$) returns $p^{[\delta-1]}$
      ii. $p^{[d-k+1]:\langle 1,j_{k+1}:j_d\rangle}$ = **iterate**($d-k+2$, d, $\boldsymbol{x}$, $(j_k=1,j_{k+1},\dots,j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      iii. $p^{[d-k+1]:\langle 2,j_{k+1}:j_d\rangle}$ = **iterate**($d-k+2$, d, $\boldsymbol{x}$, $(j_k=2,j_{k+1},\dots,j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      iv. $p^{[d-k+1]:\langle 3,j_{k+1}:j_d\rangle}$ = **iterate**($d-k+2$, d, $\boldsymbol{x}$, $(j_k=3,j_{k+1},\dots,j_d)$, $p^{[d]:\langle 1:d\rangle}$)
      v. return $\partial f\left(x_k; p^{[d-k+1]:\langle 0,j_{k+1}:j_d\rangle}, p^{[d-k+1]:\langle 1,j_{k+1}:j_d\rangle}, p^{[d-k+1]:\langle 2,j_{k+1}:j_d\rangle}, p^{[d-k+1]:\langle 3,j_{k+1}:j_d\rangle}\right)/\partial x_k$

   (b) else: // Recurse using (27)
      i. $\partial p^{[\delta]:\langle 0,d-\delta+2:d\rangle}/\partial x_k$ = **iterate_deriv**($\delta+1$,k,d,$\boldsymbol{x}$,$(j_{k+1},\dots,j_{d-\delta+1}=0,\dots,j_d)$,$p^{[d]:\langle 1:d\rangle}$)
      ii. $\partial p^{[\delta]:\langle 1,d-\delta+2:d\rangle}/\partial x_k$ = **iterate_deriv**($\delta+1$,k,d,$\boldsymbol{x}$,$(j_{k+1},\dots,j_{d-\delta+1}=1,\dots,j_d)$,$p^{[d]:\langle 1:d\rangle}$)
      iii. $\partial p^{[\delta]:\langle 2,d-\delta+2:d\rangle}/\partial x_k$ = **iterate_deriv**($\delta+1$,k,d,$\boldsymbol{x}$,$(j_{k+1},\dots,j_{d-\delta+1}=2,\dots,j_d)$,$p^{[d]:\langle 1:d\rangle}$)
      iv. $\partial p^{[\delta]:\langle 3,d-\delta+2:d\rangle}/\partial x_k$ = **iterate_deriv**($\delta+1$,k,d,$\boldsymbol{x}$,$(j_{k+1},\dots,j_{d-\delta+1}=3,\dots,j_d)$,$p^{[d]:\langle 1:d\rangle}$)
      v. return $\sum_{j_{d-\delta+1}=0}^{3} \frac{\partial f(x_{d-\delta+1})}{\partial p_{j_{d-\delta+1}}} \frac{\partial p^{[\delta]:\langle d-\delta+1:d\rangle}}{\partial x_k}$ // = right side of (27)

2. To start: **iterate_deriv**(1,k,d,$\boldsymbol{x}$,$(j_{k+1},\dots,j_d)$,$p^{[d]:\langle 1:d\rangle}$)