Spline Interpolation Method

Chemical Engineering Majors

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Transforming Numerical Methods Education for STEM Undergraduates
Spline Method of Interpolation

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What is Interpolation?

Given \((x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)\), find the value of ‘y’ at a value of ‘x’ that is not given.
Interpolants

Polynomials are the most common choice of interpolants because they are easy to:

- Evaluate
- Differentiate, and
- Integrate.
Why Splines?

\[ f(x) = \frac{1}{1 + 25x^2} \]

Table: Six equidistantly spaced points in [-1, 1]

<table>
<thead>
<tr>
<th>x</th>
<th>( y = \frac{1}{1 + 25x^2} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>-1.0</td>
<td>0.038461</td>
</tr>
<tr>
<td>-0.6</td>
<td>0.1</td>
</tr>
<tr>
<td>-0.2</td>
<td>0.5</td>
</tr>
<tr>
<td>0.2</td>
<td>0.5</td>
</tr>
<tr>
<td>0.6</td>
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Figure: 5th order polynomial vs. exact function
Why Splines?

Figure: Higher order polynomial interpolation is a bad idea
Linear Interpolation

Given \((x_0, y_0), (x_1, y_1), \ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)\), fit linear splines to the data. This simply involves forming the consecutive data through straight lines. So if the above data is given in an ascending order, the linear splines are given by \(y_i = f(x_i)\)

**Figure : Linear splines**
Linear Interpolation (contd)

\[ f(x) = f(x_0) + \frac{f(x_1) - f(x_0)}{x_1 - x_0}(x - x_0), \quad x_0 \leq x \leq x_1 \]

\[ = f(x_1) + \frac{f(x_2) - f(x_1)}{x_2 - x_1}(x - x_1), \quad x_1 \leq x \leq x_2 \]

\[ \ldots \]

\[ = f(x_{n-1}) + \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}(x - x_{n-1}), \quad x_{n-1} \leq x \leq x_n \]

Note the terms of

\[ \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \]

in the above function are simply slopes between \( x_{i-1} \) and \( x_i \).
Example

To find how much heat is required to bring a kettle of water to its boiling point, you are asked to calculate the specific heat of water at 61°C. The specific heat of water is given as a function of time in Table 1. Use linear spline interpolation to determine the value of the specific heat at $T = 61^\circ\text{C}$.

**Table 1** Specific heat of water as a function of temperature.

<table>
<thead>
<tr>
<th>Temperature, $T$ ($^\circ\text{C}$)</th>
<th>Specific heat, $C_p$ ($\frac{\text{J}}{\text{kg} \cdot ^\circ\text{C}}$)</th>
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<tbody>
<tr>
<td>22</td>
<td>4181</td>
</tr>
<tr>
<td>42</td>
<td>4179</td>
</tr>
<tr>
<td>52</td>
<td>4186</td>
</tr>
<tr>
<td>82</td>
<td>4199</td>
</tr>
<tr>
<td>100</td>
<td>4217</td>
</tr>
</tbody>
</table>

*Figure 2* Specific heat of water vs. temperature.
Linear Interpolation

\[ T_0 = 52, \quad C_p(T_0) = 4186 \]
\[ T_1 = 82, \quad C_p(T_1) = 4199 \]
\[
C_p(T) = C_p(T_0) + \frac{C_p(T_1) - C_p(T_0)}{T_1 - T_0} (T - T_0)
\]
\[ = 4186 + \frac{4199 - 4186}{82 - 52} (T - 52) \]
\[
C_p(T) = 4186 + 0.43333(T - 52), \quad 52 \leq T \leq 82
\]

At \( T = 61 \),
\[
C_p(61) = 4186 + 0.43333(61 - 52)
\]
\[ = 4189.9 \frac{J}{kg \cdot ^\circ C} \]
Quadratic Interpolation

Given \((x_0, y_0), (x_1, y_1), \ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)\), fit quadratic splines through the data. The splines are given by

\[
\begin{align*}
f(x) &= a_1 x^2 + b_1 x + c_1, \quad x_0 \leq x \leq x_1 \\
&= a_2 x^2 + b_2 x + c_2, \quad x_1 \leq x \leq x_2 \\
&\quad \vdots \\
&= a_n x^2 + b_n x + c_n, \quad x_{n-1} \leq x \leq x_n
\end{align*}
\]

Find \(a_i, b_i, c_i, i = 1, 2, \ldots, n\)
Quadratic Interpolation (contd)

Each quadratic spline goes through two consecutive data points

\[ a_1 x_0^2 + b_1 x_0 + c_1 = f(x_0) \]
\[ a_1 x_1^2 + b_1 x_1 + c_1 = f(x_1) \]
\[ a_2 x_2^2 + b_2 x_2 + c_2 = f(x_2) \]
\[ a_3 x_3^2 + b_3 x_3 + c_3 = f(x_3) \]
\[ \vdots \]
\[ a_{n-1} x_{n-1}^2 + b_{n-1} x_{n-1} + c_{n-1} = f(x_{n-1}) \]
\[ a_n x_n^2 + b_n x_n + c_n = f(x_n) \]

This condition gives 2n equations
Quadratic Splines (contd)

The first derivatives of two quadratic splines are continuous at the interior points. For example, the derivative of the first spline

\[ a_1 x^2 + b_1 x + c_1 \] is \[ 2a_1 x + b_1 \]

The derivative of the second spline

\[ a_2 x^2 + b_2 x + c_2 \] is \[ 2a_2 x + b_2 \]

and the two are equal at \( x = x_1 \) giving

\[ 2a_1 x_1 + b_1 = 2a_2 x_1 + b_2 \]

\[ 2a_1 x_1 + b_1 - 2a_2 x_1 - b_2 = 0 \]
Similarly at the other interior points,
\[ 2a_2x_2 + b_2 - 2a_3x_2 - b_3 = 0 \]
\[ . \]
\[ . \]
\[ 2a_ix_i + b_i - 2a_{i+1}x_i - b_{i+1} = 0 \]
\[ . \]
\[ . \]
\[ 2a_{n-1}x_{n-1} + b_{n-1} - 2a_nx_{n-1} - b_n = 0 \]

We have \((n-1)\) such equations. The total number of equations is \((2n) + (n - 1) = (3n - 1)\).

We can assume that the first spline is linear, that is \(a_1 = 0\)
Quadratic Splines (contd)

This gives us ‘3n’ equations and ‘3n’ unknowns. Once we find the ‘3n’ constants, we can find the function at any value of ‘x’ using the splines,

\[ f(x) = a_1 x^2 + b_1 x + c_1, \quad x_0 \leq x \leq x_1 \]

\[ = a_2 x^2 + b_2 x + c_2, \quad x_1 \leq x \leq x_2 \]

\[ \ldots \]

\[ = a_n x^2 + b_n x + c_n, \quad x_{n-1} \leq x \leq x_n \]
To find how much heat is required to bring a kettle of water to its boiling point, you are asked to calculate the specific heat of water at 61°C. The specific heat of water is given as a function of time in Table 1. Use quadratic spline interpolation to determine the value of the specific heat at $T = 61^\circ C$.

Table 1 Specific heat of water as a function of temperature.

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<td>82</td>
<td>4199</td>
</tr>
<tr>
<td>100</td>
<td>4217</td>
</tr>
</tbody>
</table>

Figure 2 Specific heat of water vs. temperature.
Solution

Since there are five data points, four quadratic splines pass through them.

\[ C_p (T) = a_1 T^2 + b_1 T + c_1, \quad 22 \leq T \leq 42 \]
\[ = a_2 T^2 + b_2 T + c_2, \quad 42 \leq T \leq 52 \]
\[ = a_3 T^2 + b_3 T + c_3, \quad 52 \leq T \leq 82 \]
\[ = a_4 T^2 + b_4 T + c_4, \quad 82 \leq T \leq 100 \]
Setting up the equations

Each quadratic spline passes through two consecutive data points giving

\[ a_i T^2 + b_i T + c_i \] passes through \( T = 22 \) and \( T = 42 \),

\[ a_1 (22)^2 + b_1 (22) + c_1 = 4181 \] \hspace{1cm} (1)

\[ a_1 (42)^2 + b_1 (42) + c_1 = 4179 \] \hspace{1cm} (2)

Similarly,

\[ a_2 (42)^2 + b_2 (42) + c_2 = 4179 \] \hspace{1cm} (3)

\[ a_2 (52)^2 + b_2 (52) + c_2 = 4186 \] \hspace{1cm} (4)

\[ a_3 (52)^2 + b_3 (52) + c_3 = 4186 \] \hspace{1cm} (5)

\[ a_3 (82)^2 + b_3 (82) + c_3 = 4199 \] \hspace{1cm} (6)

\[ a_4 (82)^2 + b_4 (82) + c_4 = 4199 \] \hspace{1cm} (7)

\[ a_4 (100)^2 + b_4 (100) + c_4 = 4217 \] \hspace{1cm} (8)
Solution (contd)

Quadratic splines have continuous derivatives at the interior data points

At $T = 42$

$$2a_1(42) + b_1 - 2a_2(42) - b_2 = 0 \quad (9)$$

At $T = 52$

$$2a_2(52) + b_2 - 2a_3(52) - b_3 = 0 \quad (10)$$

At $T = 82$

$$2a_3(82) + b_3 - 2a_4(82) - b_4 = 0 \quad (11)$$

Assuming the first spline $a_1T^2 + b_1T + c_1$ is linear,

$$a_1 = 0$$
Solution (contd)

\[
\begin{bmatrix}
484 & 22 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1764 & 42 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1764 & 42 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 2704 & 52 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 2704 & 52 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 6724 & 82 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6724 & 82 & 1 & 0 \\
84 & 1 & 0 & -84 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 104 & 1 & 0 & -104 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 164 & 1 & 0 & -164 & -1 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\end{bmatrix}
\begin{bmatrix}
a_1 \\
b_1 \\
c_1 \\
a_2 \\
b_2 \\
c_2 \\
a_3 \\
b_3 \\
c_3 \\
a_4 \\
b_4 \\
c_4 \\
\end{bmatrix}
= 
\begin{bmatrix}
4181 \\
4179 \\
4179 \\
4186 \\
4186 \\
4199 \\
4199 \\
4217 \\
0 \\
0 \\
0 \\
0 \\
0 \\
0 \\
\end{bmatrix}
\]
Solving the above 12 equations gives the 12 unknowns as

<table>
<thead>
<tr>
<th>i</th>
<th>$a_i$</th>
<th>$b_i$</th>
<th>$c_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>-0.1</td>
<td>4183.2</td>
</tr>
<tr>
<td>2</td>
<td>0.08</td>
<td>-6.82</td>
<td>4324.3</td>
</tr>
<tr>
<td>3</td>
<td>-0.035556</td>
<td>5.1978</td>
<td>4011.9</td>
</tr>
<tr>
<td>4</td>
<td>0.090741</td>
<td>-15.515</td>
<td>4861.1</td>
</tr>
</tbody>
</table>
Therefore, the splines are given by

\[ C_p(T) = -0.1T + 4183.2, \quad 22 \leq T \leq 42 \]
\[ = 0.08T^2 - 6.82T + 4324.3, \quad 42 \leq T \leq 52 \]
\[ = -0.035556T^2 + 5.1978T + 4011.9, \quad 52 \leq T \leq 82 \]
\[ = 0.090741T^2 - 15.515T + 4861.1, \quad 82 \leq T \leq 100 \]

At \( T = 61 \)

\[ C_p(61) = -0.035556(61)^2 + 5.1978(61) + 4011.9 \]
\[ = 4196.6 \frac{J}{kg \cdot ^\circ C} \]

The absolute relative approximate error \( |\varepsilon_a| \) obtained between the results from the linear and quadratic splines is

\[ |\varepsilon_a| = \left| \frac{4196.6 - 4189.9}{4196.6} \right| \times 100 \]
\[ = 0.16013\% \]
Better Estimate

The heat required to heat the water is given more accurately by

\[ Q = m \int_{T_r}^{T_b} C_p \, dT \]

\( T_r = \) room temperature \( (^{\circ}C) \) \hspace{1cm} \( T_b = \) boiling temperature of water \( (^{\circ}C) \)

Given \( T_r = 22^{\circ}C \) \hspace{1cm} \( T_b = 100^{\circ}C \)

Find a better estimate of the heat required. What is the difference between the results from this method and the Quadratic Interpolation?
Better Estimate

\[ \int_{T_r}^{T_i} C_p dT = \int_{22}^{100} C_p(T) dT \]

\[ = \int_{22}^{42} C_p(T) dT + \int_{42}^{52} C_p(T) dT + \int_{52}^{82} C_p(T) dT + \int_{82}^{100} C_p(T) dT \]

\[ = \int_{22}^{42} (-0.1T + 4183.2) dT + \int_{42}^{52} (0.08T^2 - 6.82T + 4324.3) dT \]

\[ + \int_{52}^{82} (-0.035556T^2 + 5.1978T + 4011.9) dT + \int_{82}^{100} (0.090741T^2 - 15.515T + 4861.1) dT \]

\[ = \left[ -0.1 \frac{T^2}{2} + 4183.2T \right]_{22}^{42} + \left[ 0.08 \frac{T^3}{3} - 6.82 \frac{T^2}{2} + 4324.3T \right]_{42}^{52} \]

\[ + \left[ -0.035556 \frac{T^3}{3} + 5.1978 \frac{T^2}{2} + 4011.9T \right]_{52}^{82} + \left[ 0.090741 \frac{T^3}{3} - 15.515 \frac{T^2}{2} + 4861.1T \right]_{82}^{100} \]

\[ = [83600] + [41812] + [125940] + [75656] \]

\[ = 3.2700 \times 10^5 \frac{J}{kg} \]
Better Estimate

To compare this result with our results from Quadratic interpolation, we take the average specific heat over this interval, given by:

\[
C_{p,\text{avg}} = \frac{\int_{T_r}^{T_b} C_p dT}{T_b - T_r}
\]

\[
= \frac{3.2700 \times 10^5}{100 - 22}
\]

\[
= 4192.3 \frac{J}{\text{kg} \cdot ^\circ \text{C}}
\]

Knowing that this method is the more accurate way of calculating the heat transfer, we define the absolute relative approximate error \(|\varepsilon_a|\) by

\[
|\varepsilon_a| = \left| \frac{4192.3 - 4196.7}{4192.3} \right| \times 100
\]

\[
= 0.10211\%
\]
Additional Resources

For all resources on this topic such as digital audiovisual lectures, primers, textbook chapters, multiple-choice tests, worksheets in MATLAB, MATHEMATICA, MathCad and MAPLE, blogs, related physical problems, please visit

http://numericalmethods.eng.usf.edu/topics/spline_method.html
THE END

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