

Interpolation



Topic: Newton's Divided
Difference Polynomial Method

Major: Chemical



What is Interpolation ?

Given $(x_0, y_0), (x_1, y_1), \dots, (x_n, y_n)$, 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.

Newton's Divided Difference Method

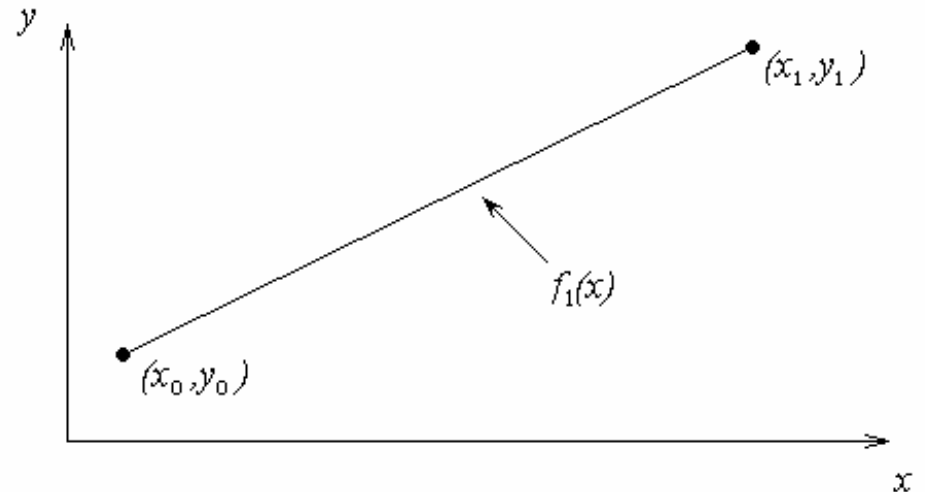
Linear interpolation: Given (x_0, y_0) , (x_1, y_1) , pass a linear interpolant through the data

$$f_1(x) = b_0 + b_1(x - x_0)$$

where

$$b_0 = f(x_0)$$

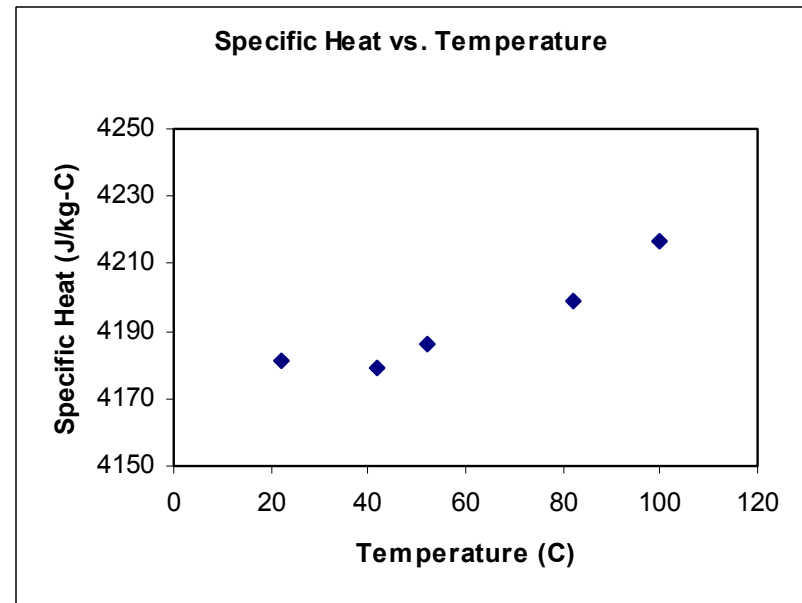
$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$



Example

To find how much heat is required to bring a kettle of water to boiling point, you are asked to calculate the specific heat of water at 61°C Use linear and quadratic interpolation.

Temperature	Specific heat
°C	$\frac{J}{kg - ^\circ C}$
22	4181
42	4179
52	4186
82	4199
100	4217



Linear Interpolation

$$C_p(T) = b_0 + b_1(T - T_0)$$

$$T_0 = 52, C_p(T_0) = 4186$$

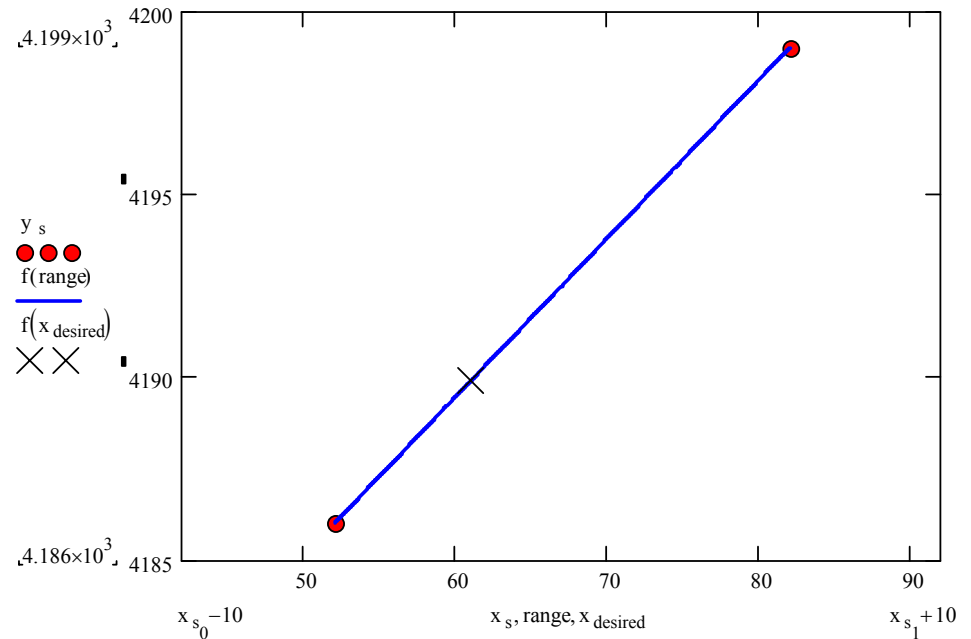
$$T_1 = 82, C_p(T_1) = 4199$$

$$b_0 = C_p(T_0) = 4186$$

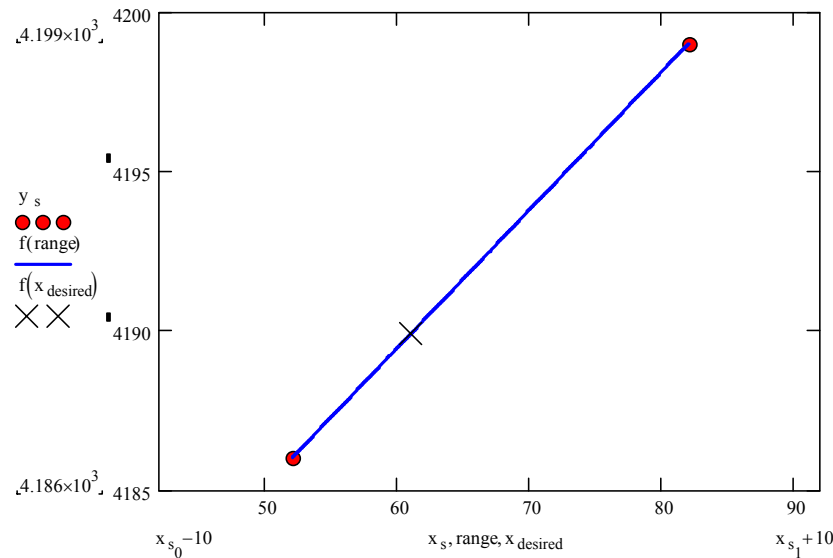
$$b_1 = \frac{C_p(T_1) - C_p(T_0)}{T_1 - T_0}$$

$$= \frac{4199 - 4186}{82 - 52}$$

$$= 0.43333$$



Linear Interpolation (contd)



$$\begin{aligned} C_p(T) &= b_0 + b_1(T - T_0) \\ &= 4186 + 0.43333(T - 52), \quad 52 \leq T \leq 82 \end{aligned}$$

At $T = 61$

$$\begin{aligned} C_p(61) &= 4186 + 0.43333(61 - 52) \\ &= 4189.9 \frac{J}{kg \cdot ^\circ C} \end{aligned}$$



Quadratic Interpolation

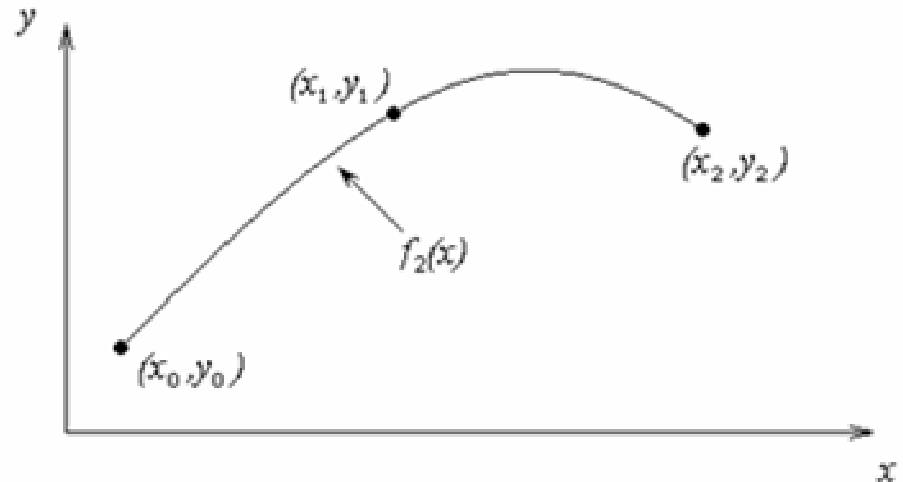
Given (x_0, y_0) , (x_1, y_1) , and (x_2, y_2) , fit a quadratic interpolant through the data.

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

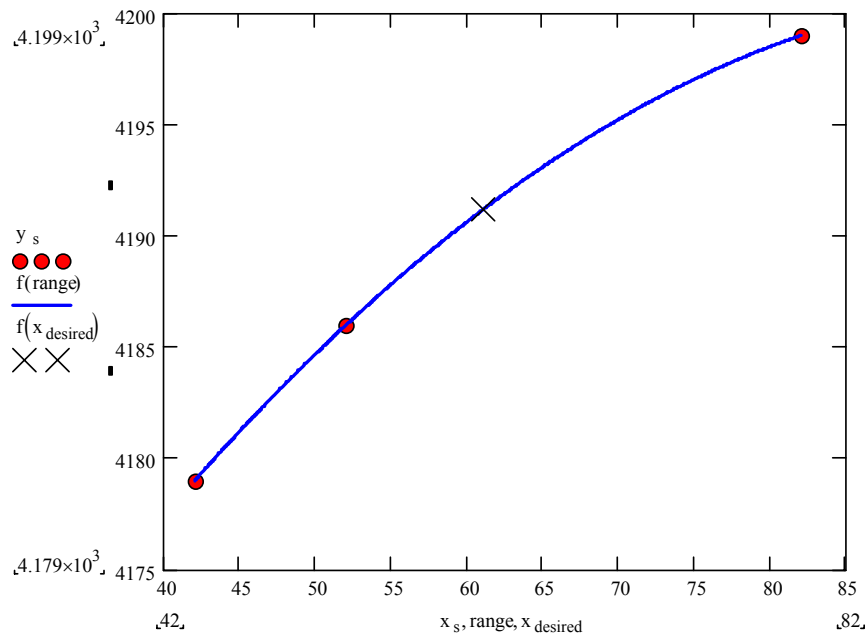
$$b_0 = f(x_0)$$

$$b_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$b_2 = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$



Quadratic Interpolation (contd)



$$C_p(T) = b_0 + b_1(T - T_0) + b_2(T - T_0)(T - T_1)$$

$$T_0 = 42, C_p(T_0) = 4179$$

$$T_1 = 52, C_p(T_1) = 4186$$

$$T_2 = 82, C_p(T_2) = 4199$$



Quadratic Interpolation (contd)

$$b_0 = C_p(T_0) = 4179$$

$$b_1 = \frac{C_p(T_1) - C_p(T_0)}{T_1 - T_0} = \frac{4186 - 4179}{52 - 42} = 0.7$$

$$\begin{aligned} b_2 &= \frac{\frac{C_p(T_2) - C_p(T_1)}{T_2 - T_1} - \frac{C_p(T_1) - C_p(T_0)}{T_1 - T_0}}{T_2 - T_0} = \frac{\frac{4199 - 4186}{82 - 52} - \frac{4186 - 4179}{52 - 42}}{82 - 42} \\ &= \frac{0.43333 - 0.7}{40} \\ &= -6.6667 * 10^{-3} \end{aligned}$$



Quadratic Interpolation (contd)

$$\begin{aligned}C_p(T) &= b_0 + b_1(T - T_0) + b_2(T - T_0)(T - T_1) \\ &= 4179 + 0.7(T - 42) - 6.6667 * 10^{-3}(T - 42)(T - 52), \quad 42 \leq T \leq 82\end{aligned}$$

At $T = 61$,

$$\begin{aligned}C_p(61) &= 4179 + 0.7(61 - 42) + 6.6667 * 10^{-3}(61 - 42)(61 - 52) \\ &= 4191.2 \frac{J}{kg - ^\circ C}\end{aligned}$$

The absolute relative approximate error $|\epsilon_a|$ obtained between the results from the first and second order polynomial is

$$\begin{aligned}|\epsilon_a| &= \left| \frac{4191.2 - 4189.9}{4191.2} \right| \times 100 \\ &= 0.031017\%\end{aligned}$$



General Form

$$f_2(x) = b_0 + b_1(x - x_0) + b_2(x - x_0)(x - x_1)$$

where

$$b_0 = f[x_0] = f(x_0)$$

$$b_1 = f[x_1, x_0] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

$$b_2 = f[x_2, x_1, x_0] = \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0} = \frac{\frac{f(x_2) - f(x_1)}{x_2 - x_1} - \frac{f(x_1) - f(x_0)}{x_1 - x_0}}{x_2 - x_0}$$

Rewriting

$$f_2(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1)$$



General Form

Given $(n + 1)$ data points, $(x_0, y_0), (x_1, y_1), \dots, (x_{n-1}, y_{n-1}), (x_n, y_n)$,

$$f_n(x) = b_0 + b_1(x - x_0) + \dots + b_n(x - x_0)(x - x_1)\dots(x - x_{n-1})$$

where

$$b_0 = f[x_0]$$

$$b_1 = f[x_1, x_0]$$

$$b_2 = f[x_2, x_1, x_0]$$

\vdots

$$b_{n-1} = f[x_{n-1}, x_{n-2}, \dots, x_0]$$

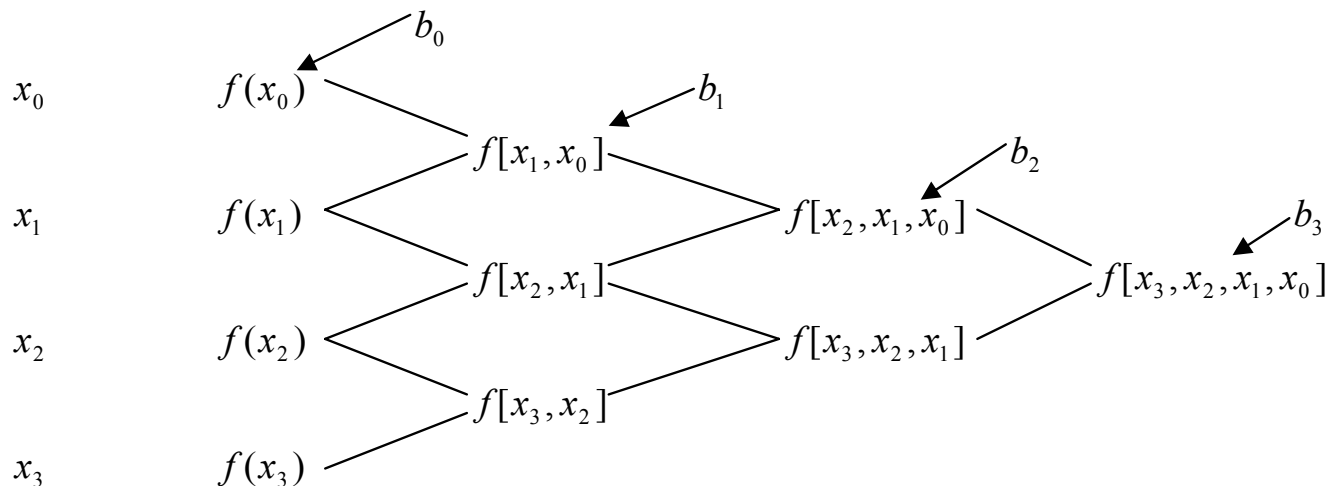
$$b_n = f[x_n, x_{n-1}, \dots, x_0]$$



General form

The third order polynomial, given (x_0, y_0) , (x_1, y_1) , (x_2, y_2) , and (x_3, y_3) , is

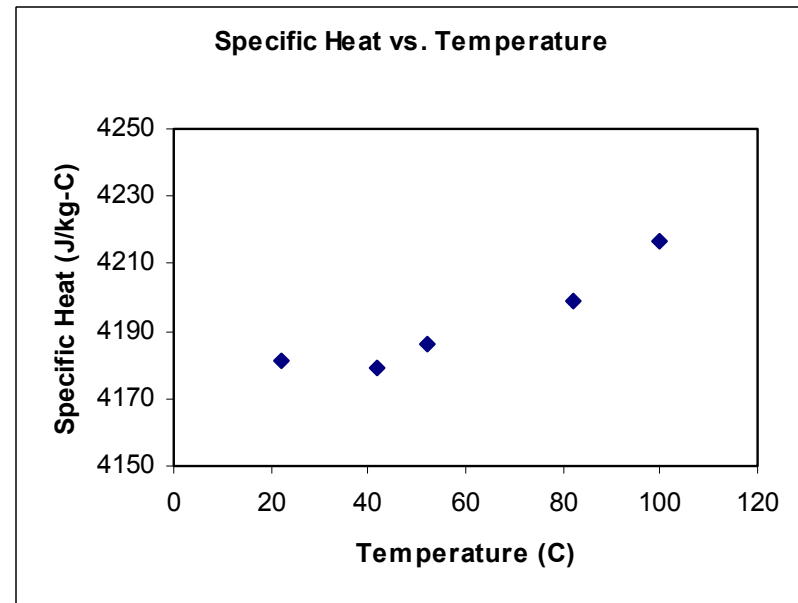
$$f_3(x) = f[x_0] + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1) + f[x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2)$$



Example

To find how much heat is required to bring a kettle of water to boiling point, you are asked to calculate the specific heat of water at 61°C . Use cubic interpolation.

Temperature	Specific heat
$^{\circ}\text{C}$	$\frac{J}{\text{kg} - ^{\circ}\text{C}}$
22	4181
42	4179
52	4186
82	4199
100	4217





Example

The specific heat profile is chosen as

$$C_p(T) = b_0 + b_1(T - T_0) + b_2(T - T_0)(T - T_1) + b_3(T - T_0)(T - T_1)(T - T_2)$$

We need to choose four data points that are closest to $T = 61^\circ\text{C}$.

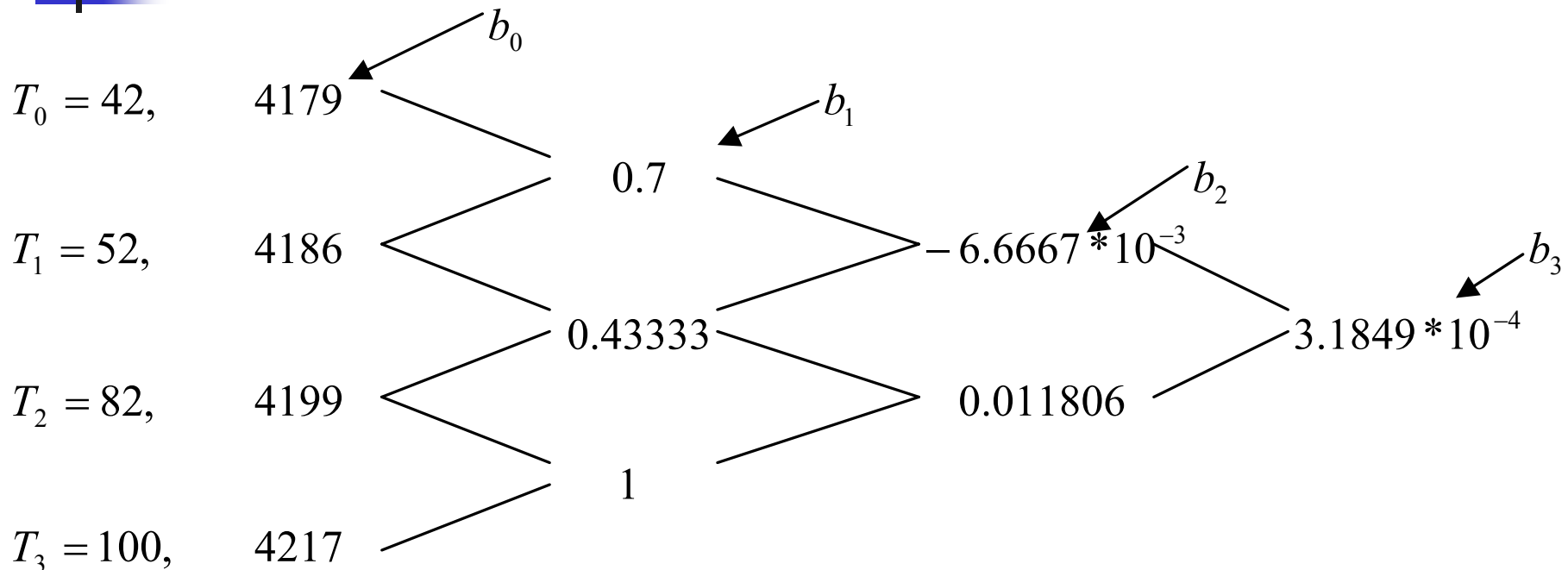
$$T_0 = 42, \quad C_p(T_0) = 4179$$

$$T_1 = 52, \quad C_p(T_1) = 4186$$

$$T_2 = 82, \quad C_p(T_2) = 4199$$

$$T_3 = 100, \quad C_p(T_3) = 4217$$

Example



The values of the constants are found to be

$$b_0 = 4179 \quad b_1 = 0.7 \quad b_2 = -6.6667 * 10^{-3} \quad b_3 = 3.1849 * 10^{-4}$$



Example

$$\begin{aligned}C_p(T) &= b_0 + b_1(T - T_0) + b_2(T - T_0)(T - T_1) + b_3(T - T_0)(T - T_1)(T - T_2) \\ &= 4179 + 0.7(T - 42) - 6.6667 * 10^{-3}(T - 42)(T - 52) \\ &\quad + 3.1849 * 10^{-4}(T - 42)(T - 52)(T - 82)\end{aligned}$$

At $T = 61$,

$$\begin{aligned}C_p(61) &= 4179 + 0.7(61 - 42) - 6.6667 * 10^{-3}(61 - 42)(61 - 52) \\ &\quad + 3.1849 * 10^{-4}(61 - 42)(61 - 52)(61 - 82) \\ &= 4190.0 \frac{J}{kg - ^\circ C}\end{aligned}$$

The absolute relative approximate error $|\epsilon_a|$ obtained between the results from the second and third order polynomial is

$$\begin{aligned}|\epsilon_a| &= \left| \frac{4190.0 - 4191.2}{4190.0} \right| \times 100 \\ &= 0.028640 \%\end{aligned}$$



Comparison Table

Order of Polynomial	1	2	3
$C_p(T)$ $\frac{J}{kg - ^\circ C}$	4189.9	4191.2	4190.0
Absolute Relative Approximate Error	-----	0.031017%	0.028640%