

Interpolation



Topic: Spline Interpolation 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.

Why Splines ?

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

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

x	$y = \frac{1}{1 + 25x^2}$
-1.0	0.038461
-0.6	0.1
-0.2	0.5
0.2	0.5
0.6	0.1
1.0	0.038461

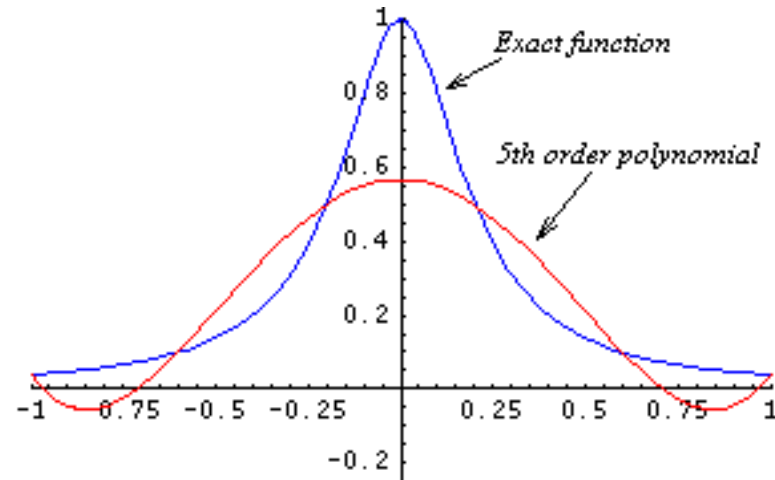


Figure : 5th order polynomial vs. exact function

Why Splines ?

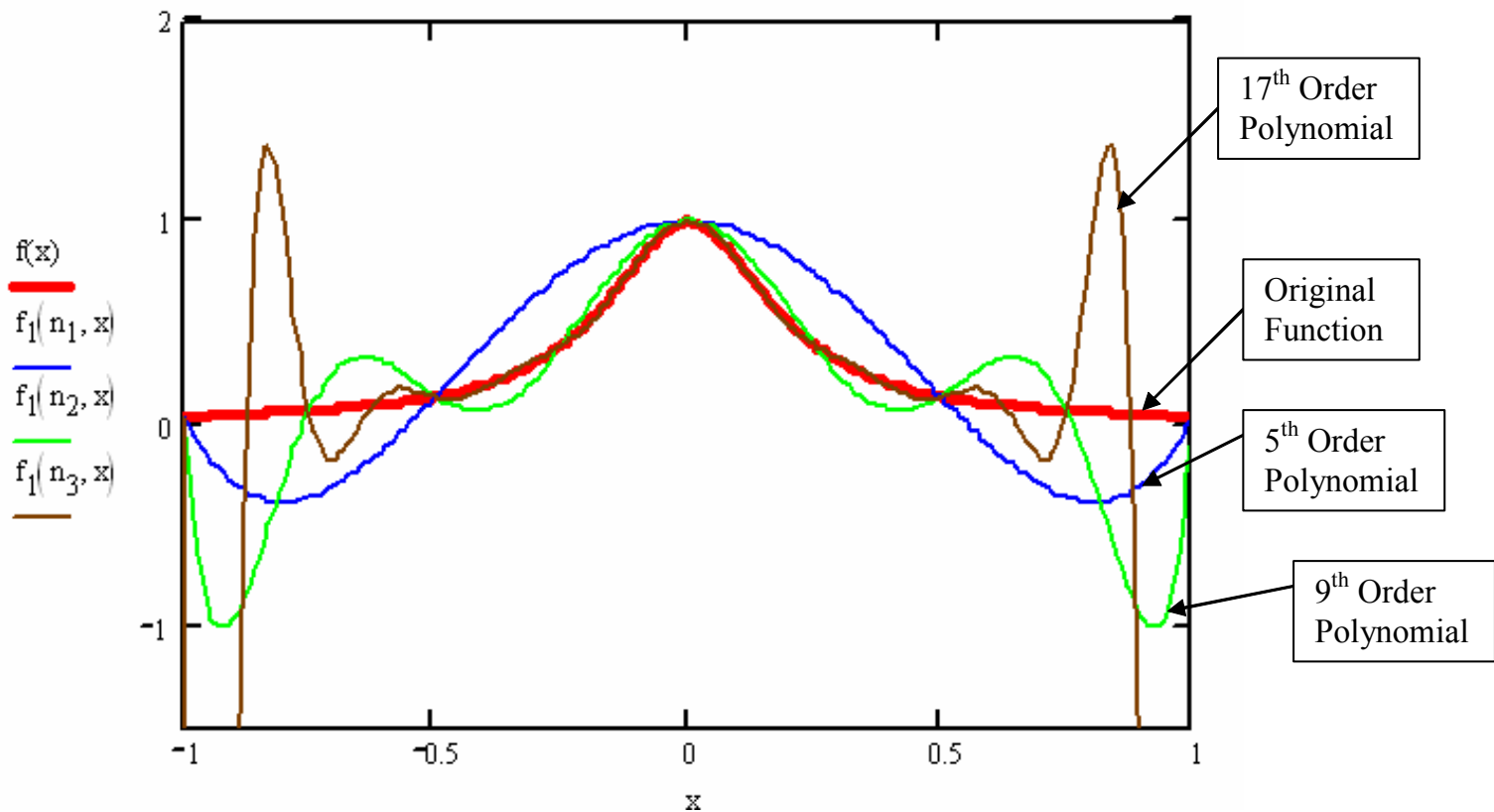


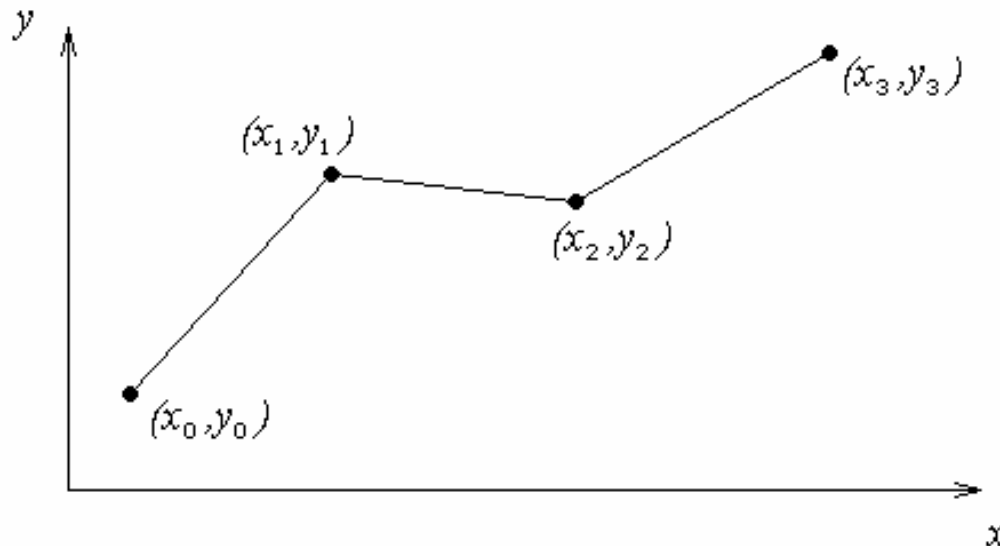
Figure : Higher order polynomial interpolation is a bad idea



Linear Interpolation

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

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

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

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

Note the terms of

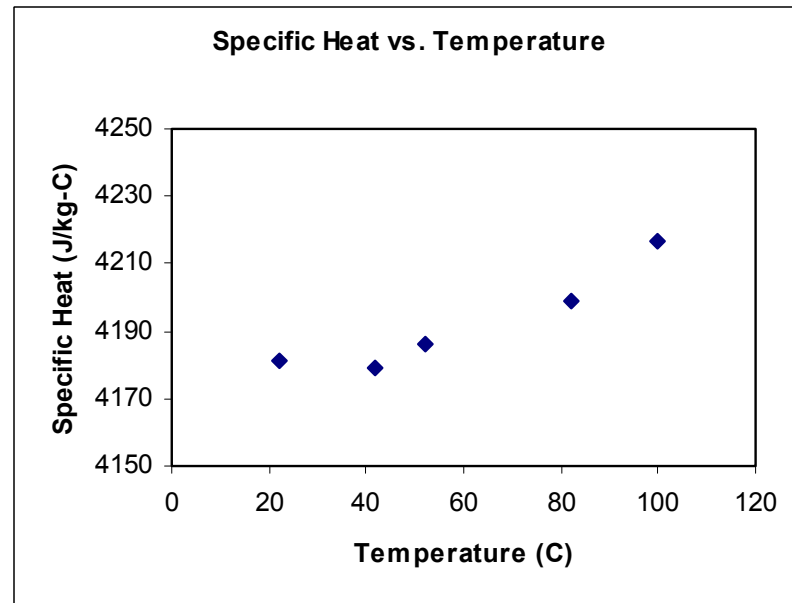
$$\frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

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 boiling point, you are asked to calculate the specific heat of water at 61°C. Use linear spline interpolation.

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



Linear Interpolation

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

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

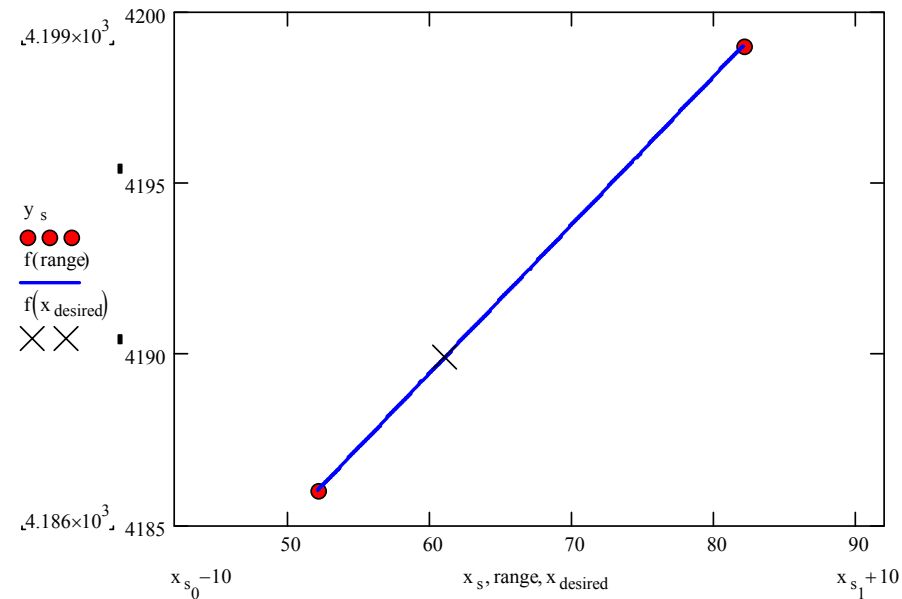
$$\begin{aligned} C_p(T) &= C_p(T_0) + \frac{C_p(T_1) - C_p(T_0)}{T_1 - T_0} (T - T_0) \\ &= 4186 + \frac{4199 - 4186}{82 - 52} (T - 52) \end{aligned}$$

$$C_p(T) = 4186 + 0.43333(T - 52)$$

At $T = 61$,

$$C_p(61) = 4186 + 0.43333(61 - 52)$$

$$= 4189.9 \frac{J}{kg \cdot ^\circ C}$$



Quadratic Interpolation

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

$$f(x) = a_1x^2 + b_1x + c_1, \quad x_0 \leq x \leq x_1$$

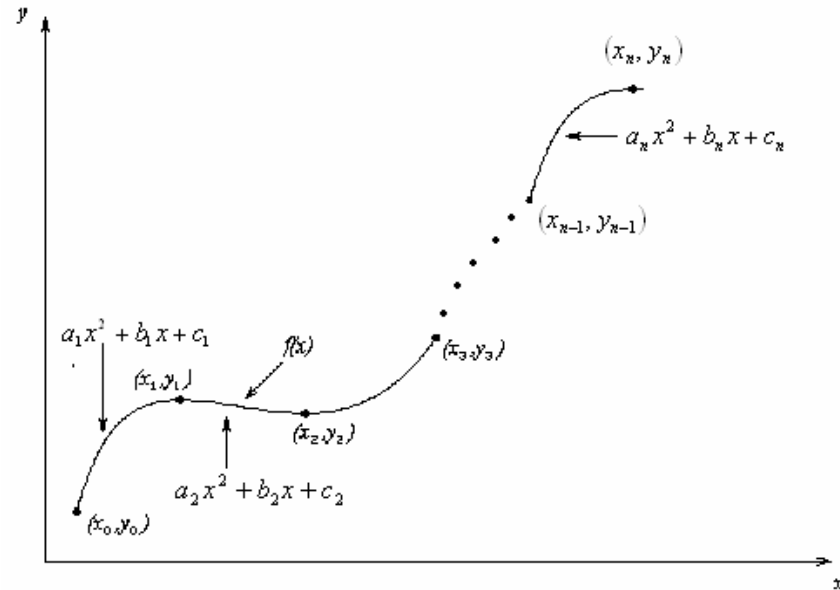
$$= a_2x^2 + b_2x + c_2, \quad x_1 \leq x \leq x_2$$

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$$= a_nx^2 + b_nx + c_n, \quad x_{n-1} \leq x \leq x_n$$

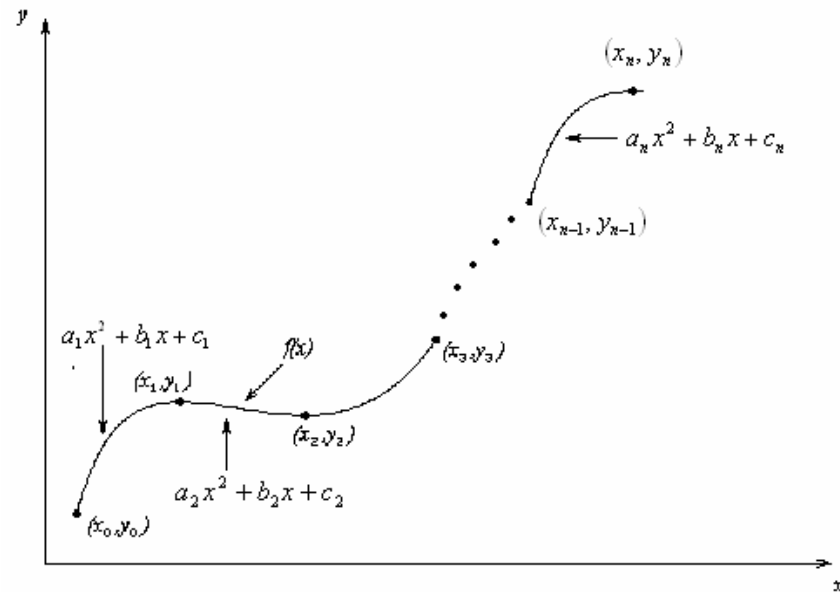


Find $a_i, b_i, c_i, i = 1, 2, \dots, n$

Quadratic Interpolation (contd)

Each quadratic spline goes through two consecutive data points

$$\begin{aligned}
 a_1 x_0^2 + b_1 x_0 + c_1 &= f(x_0) \\
 a_1 x_1^2 + b_1 x_1 + c_1 &= f(x_1) \\
 &\vdots \\
 a_i x_{i-1}^2 + b_i x_{i-1} + c_i &= f(x_{i-1}) \\
 a_i x_i^2 + b_i x_i + c_i &= f(x_i) \\
 &\vdots \\
 a_n x_{n-1}^2 + b_n x_{n-1} + c_n &= f(x_{n-1}) \\
 a_n x_n^2 + b_n x_n + c_n &= f(x_n)
 \end{aligned}$$



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

$$a_1x^2 + b_1x + c_1 \text{ is } 2a_1x + b_1$$

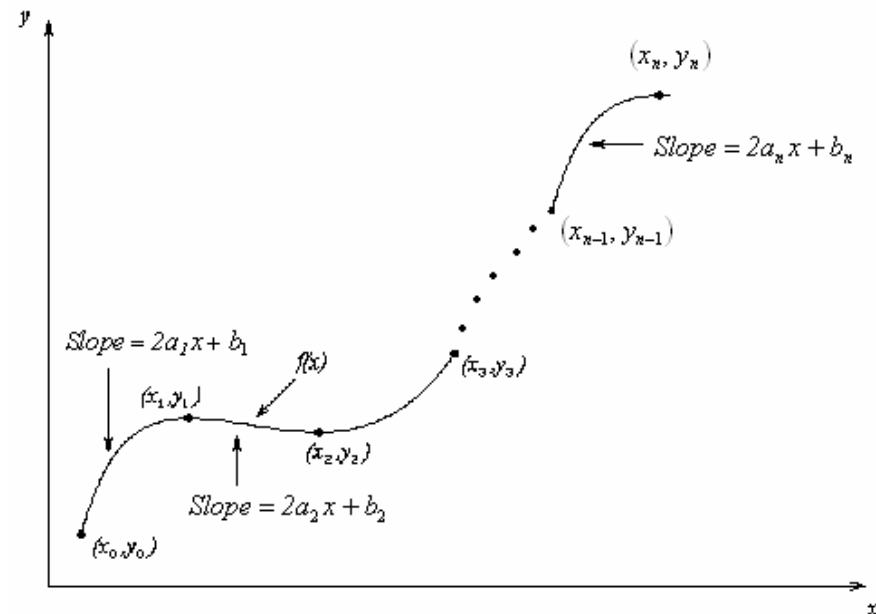
The derivative of the second spline

$$a_2x^2 + b_2x + c_2 \text{ is } 2a_2x + b_2$$

and the two are equal at $x = x_1$ giving

$$2a_1x_1 + b_1 = 2a_2x_1 + b_2$$

$$2a_1x_1 + b_1 - 2a_2x_1 - b_2 = 0$$



Quadratic Splines (contd)

Similarly at the other interior points,

$$2a_2x_2 + b_2 - 2a_3x_2 - b_3 = 0$$

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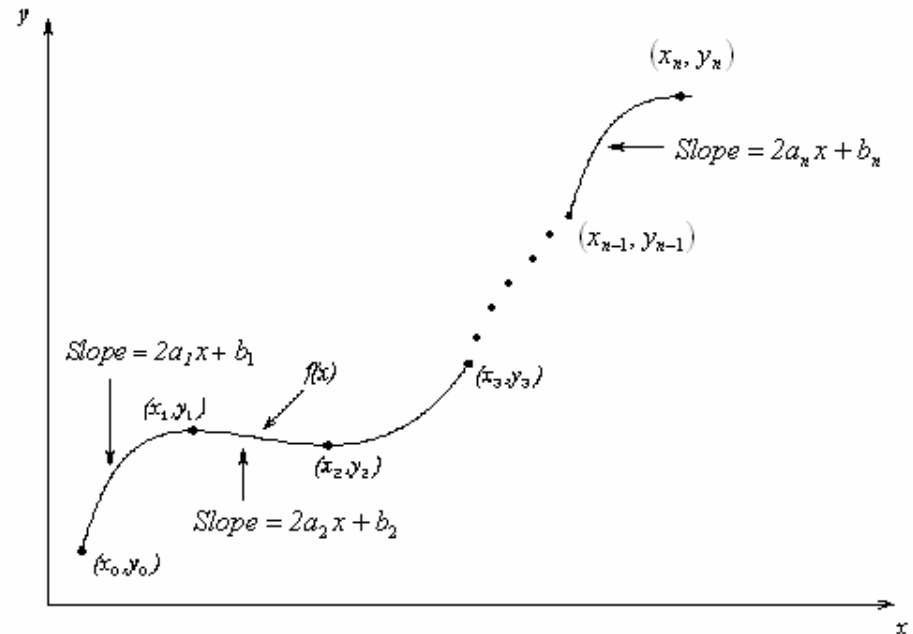
$$2a_ix_i + b_i - 2a_{i+1}x_i - b_{i+1} = 0$$

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$$2a_{n-1}x_{n-1} + b_{n-1} - 2a_nx_{n-1} - b_n = 0$$



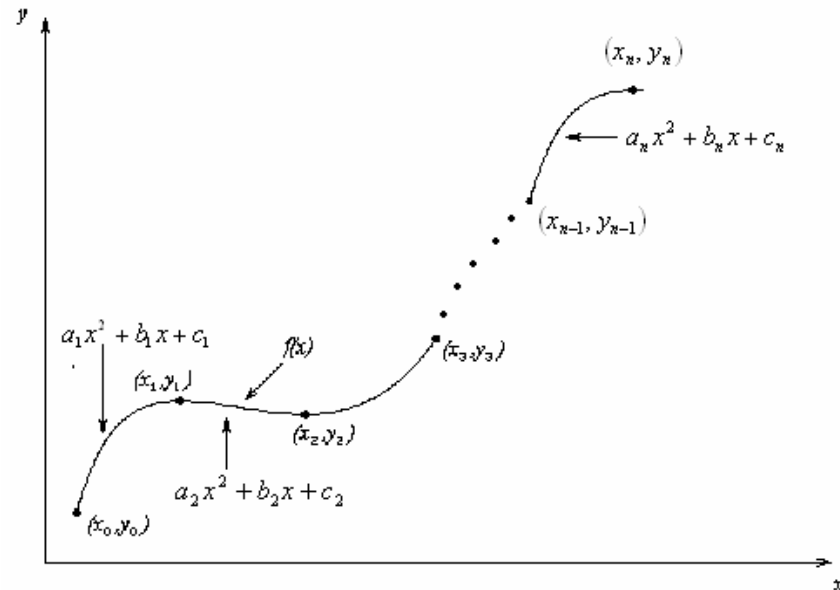
We have (n-1) such equations. The total number of equations is $(2n) + (n - 1) = (3n - 1)$.

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,

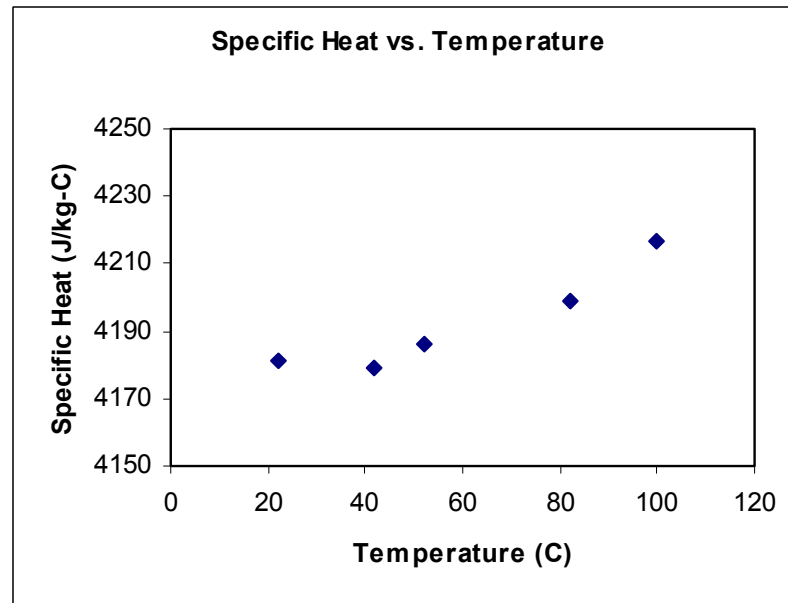
$$\begin{aligned}
 f(x) &= a_1x^2 + b_1x + c_1, & x_0 \leq x \leq x_1 \\
 &= a_2x^2 + b_2x + c_2, & x_1 \leq x \leq x_2 \\
 &\cdot \\
 &\cdot \\
 &\cdot \\
 &= a_nx^2 + b_nx + c_n, & x_{n-1} \leq x \leq x_n
 \end{aligned}$$



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 quadratic spline interpolation.

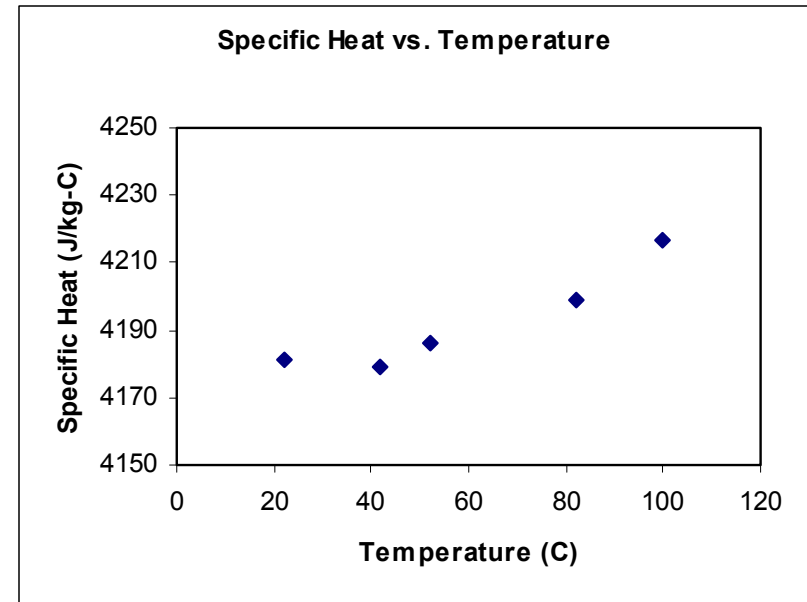
Temperature	Specific heat
°C	$\frac{J}{kg - ^\circ C}$
22	4181
42	4179
52	4186
82	4199
100	4217



Solution

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

$$\begin{aligned}C_p(T) &= a_1T^2 + b_1T + c_1, & 22 \leq T \leq 42 \\ &= a_2T^2 + b_2T + c_2, & 42 \leq T \leq 52 \\ &= a_3T^2 + b_3T + c_3, & 52 \leq T \leq 82 \\ &= a_4T^2 + b_4T + c_4, & 82 \leq T \leq 100\end{aligned}$$





Solution (contd)

Setting up the equations

Each quadratic spline passes through two consecutive data points giving

$a_1T^2 + b_1T + c_1$ passes through $T = 22$ and $T = 42$,

$$a_1(22)^2 + b_1(22) + c_1 = 4181 \quad (1)$$

$$a_1(42)^2 + b_1(42) + c_1 = 4179 \quad (2)$$

Similarly,

$$a_2(42)^2 + b_2(42) + c_2 = 4179 \quad (3)$$

$$a_2(52)^2 + b_2(52) + c_2 = 4186 \quad (4)$$

$$a_3(52)^2 + b_3(52) + c_3 = 4186 \quad (5)$$

$$a_3(82)^2 + b_3(82) + c_3 = 4199 \quad (6)$$

$$a_4(82)^2 + b_4(82) + c_4 = 4199 \quad (7)$$

$$a_4(100)^2 + b_4(100) + c_4 = 4217 \quad (8)$$

Solution (contd)

Quadratic splines have continuous derivatives at the interior data points

At $T = 42$

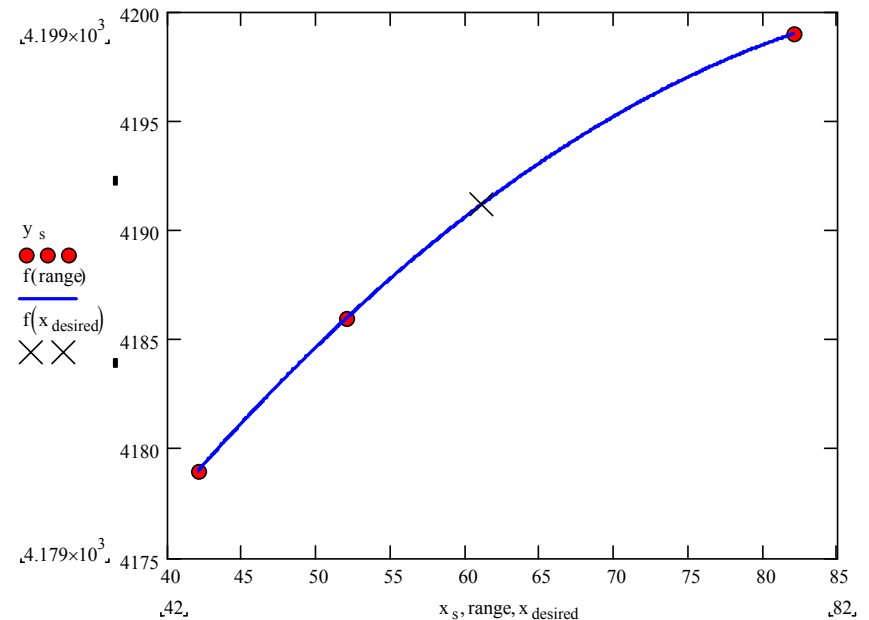
$$2a_1(42) + b_1 - 2a_2(42) - b_2 = 0 \quad (9)$$

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)

$$\begin{bmatrix}
 484 & 22 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 1764 & 42 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 1764 & 42 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 2704 & 52 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 2704 & 52 & 1 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 6724 & 82 & 1 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 6724 & 82 & 1 \\
 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 10000 & 100 & 1 \\
 84 & 1 & 0 & -84 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 104 & 1 & 0 & -104 & -1 & 0 & 0 & 0 & 0 \\
 0 & 0 & 0 & 0 & 0 & 0 & 164 & 1 & 0 & -164 & -1 & 0 \\
 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0
 \end{bmatrix}
 \begin{bmatrix}
 a_1 \\
 b_1 \\
 c_1 \\
 a_2 \\
 b_2 \\
 c_2 \\
 a_3 \\
 b_3 \\
 c_3 \\
 a_4 \\
 b_4 \\
 c_4
 \end{bmatrix}
 =
 \begin{bmatrix}
 4181 \\
 4179 \\
 4179 \\
 4186 \\
 4186 \\
 4199 \\
 4199 \\
 4217 \\
 0 \\
 0 \\
 0 \\
 0
 \end{bmatrix}$$



Solution (contd)

Solving the above 12 equations gives the 12 unknowns as

i	a_i	b_i	c_i
1	0	-0.1	4183.2
2	0.08	-6.82	4324.3
3	-0.035556	5.1978	4011.9
4	0.090741	-15.515	4861.1

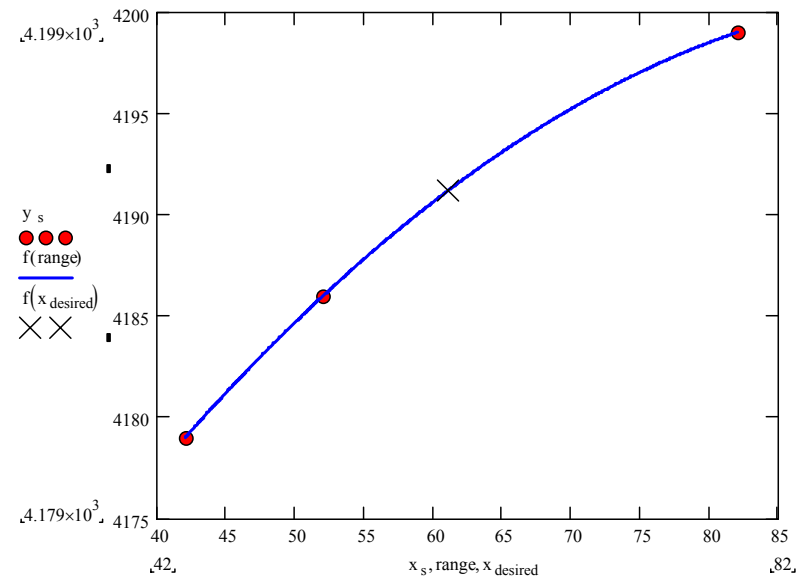
Solution (contd)

Therefore, the splines are given by

$$\begin{aligned}
 C_p(T) &= -0.1T + 4183.2, & 22 \leq T \leq 42 \\
 &= 0.08T^2 - 6.82T + 4324.3, & 42 \leq T \leq 52 \\
 &= -0.035556T^2 + 5.1978T + 4011.9, & 52 \leq T \leq 82 \\
 &= 0.090741T^2 - 15.515T + 4861.1, & 82 \leq T \leq 100
 \end{aligned}$$

At $T = 61$

$$\begin{aligned}
 C_p(61) &= -0.035556(61)^2 + 5.1978(61) + 4011.9 \\
 &= 4196.7 \frac{J}{kg - ^\circ C}
 \end{aligned}$$



The absolute relative approximate error $|\epsilon_a|$ obtained between the results from the linear and quadratic splines is

$$\begin{aligned}
 |\epsilon_a| &= \left| \frac{4196.7 - 4189.9}{4196.7} \right| \times 100 \\
 &= 0.16203\%
 \end{aligned}$$



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 ($^{\circ}C$)

T_b = boiling temperature of water ($^{\circ}C$)

Given $T_r = 22^{\circ}C$

$T_b = 100^{\circ}C$

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



Better Estimate

$$\int_{T_r}^{T_b} C_p dT = \int_{22}^{100} C_p(T) dT$$

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

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

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

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

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

$$= [83600] + [41811] + [125936] + [75656]$$

$$= 3.2700 * 10^5 \frac{J}{kg}$$



Better Estimate

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

$$\begin{aligned}C_{p,ave} &= \frac{\int_{T_r}^{T_b} C_p dT}{T_b - T_r} \\ &= \frac{3.2700 * 10^5}{100 - 22} \\ &= 4192.3 \frac{J}{kg - ^\circ C}\end{aligned}$$

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

$$\begin{aligned}|\epsilon_a| &= \left| \frac{4192.3 - 4196.7}{4192.3} \right| \times 100 \\ &= 0.10495\%\end{aligned}$$