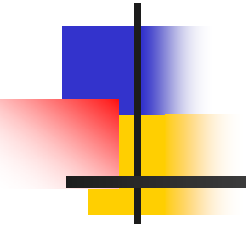




Differentiation-Discrete Functions



Major: Chemical Engineering

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Forward Difference Approximation

$$f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

For a finite ' Δx '

$$f'(x) \cong \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

Graphical Representation Of Forward Difference Approximation

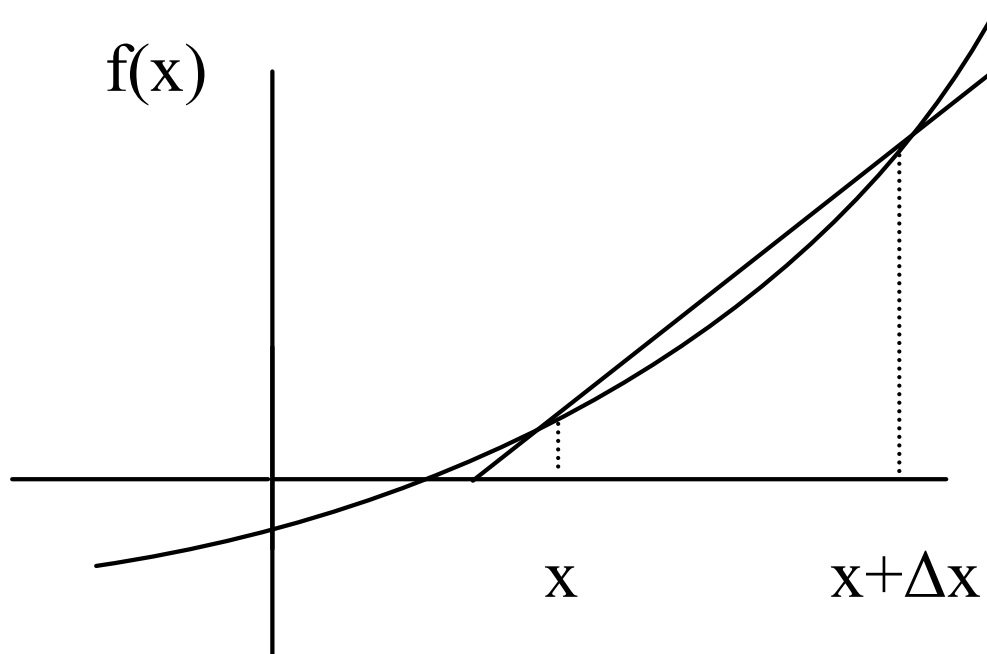


Figure 1: Graphical Representation of forward difference approximation of first derivative



Example 1

A new fuel for recreational boats being developed at the local university was tested at an area pond by a team of engineers. The interest is to document the environmental impact of the fuel – how quickly does the slick spread? The table below shows the video camera record of the radius of the wave generated by a drop of the fuel that fell into the pond. Using the data

- a) Compute the rate at which the radius of the drop was changing at $t = 2$.
- b) Estimate the rate at which the area of the contaminant was spreading across the pond at $t = 2$.



Example 1 Cont.

Time (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Radius (m)	0	0.236	0.667	1.225	1.886	2.635	3.464	4.365	5.333

Use Forward Divided Difference approximation of the first derivative to solve the above problem. Use a time step of 0.5 sec.



Example 1 Cont.

Solution

$$(a) \quad R'(t_i) \cong \frac{R(t_{i+1}) - R(t_i)}{\Delta t}$$

$$t_i = 2$$

$$\Delta t = 0.5$$

$$t_{i+1} = t_i + \Delta t$$

$$t_{i+1} = 2 + 0.5 = 2.5$$

$$R'(2) = \frac{R(2.5) - R(2)}{0.5}$$

$$= \frac{2.635 - 1.886}{0.5}$$

$$= 1.498m/sec$$



Example 1 Cont.

(b) $Area = \pi R^2$

Time (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Area(m ²)	0	0.175	1.398	4.714	11.17	21.81	37.69	67.49	89.35

$$A'(t_i) \cong \frac{A(t_{i+1}) - A(t_i)}{\Delta t}$$

$$t_i = 2$$

$$\Delta t = 0.5$$

$$t_{i+1} = t_i + \Delta t$$



Example 1 Cont.

$$t_{i+1} = 2 + 0.5 = 2.5$$

$$\begin{aligned} A'(10) &= \frac{A(2.5) - A(2)}{0.5} \\ &= \frac{21.81 - 11.17}{0.5} \\ &= 21.28m^2 / \text{sec} \end{aligned}$$



Direct Fit Polynomials

In this method, given ' $n+1$ ' data points $(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$

, one can fit a n^{th} order polynomial given by

$$P_n(x) = a_0 + a_1x + \dots + a_{n-1}x^{n-1} + a_nx^n$$

To find the first derivative,

$$P'_n(x) = \frac{dP_n(x)}{dx} = a_1 + 2a_2x + \dots + (n-1)a_{n-1}x^{n-2} + na_nx^{n-1}$$

Similarly other derivatives can be found.



Example 2-Direct Fit Polynomials

A new fuel for recreational boats being developed at the local university was tested at an area pond by a team of engineers. The interest is to document the environmental impact of the fuel – how quickly does the slick spread? The table below shows the video camera record of the radius of the wave generated by a drop of the fuel that fell into the pond. Using the data

- (a) Compute the rate at which the radius of the drop was changing at $t = 2$.
- (b) Estimate the rate at which the area of the contaminant was spreading across the pond at $t = 2$.

Time (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Radius (m)	0	0.236	0.667	1.225	1.886	2.635	3.464	4.365	5.333

Use the third order polynomial interpolant for Radius and Area.



Example 2-Direct Fit Polynomials cont.

Solution

(a) For the third order polynomial (also called cubic interpolation), we choose the radius given by

$$R(t) = a_0 + a_1t + a_2t^2 + a_3t^3$$

Since we want to find the radius at $t=2$, and we are using a third order polynomial, we need to choose the four points closest to $t=2$ and that also bracket $t=2$ to evaluate it.

The four points are $t_0=1.0$, $t_1=1.5$, $t_2=2.0$ and $t_3=2.5$.

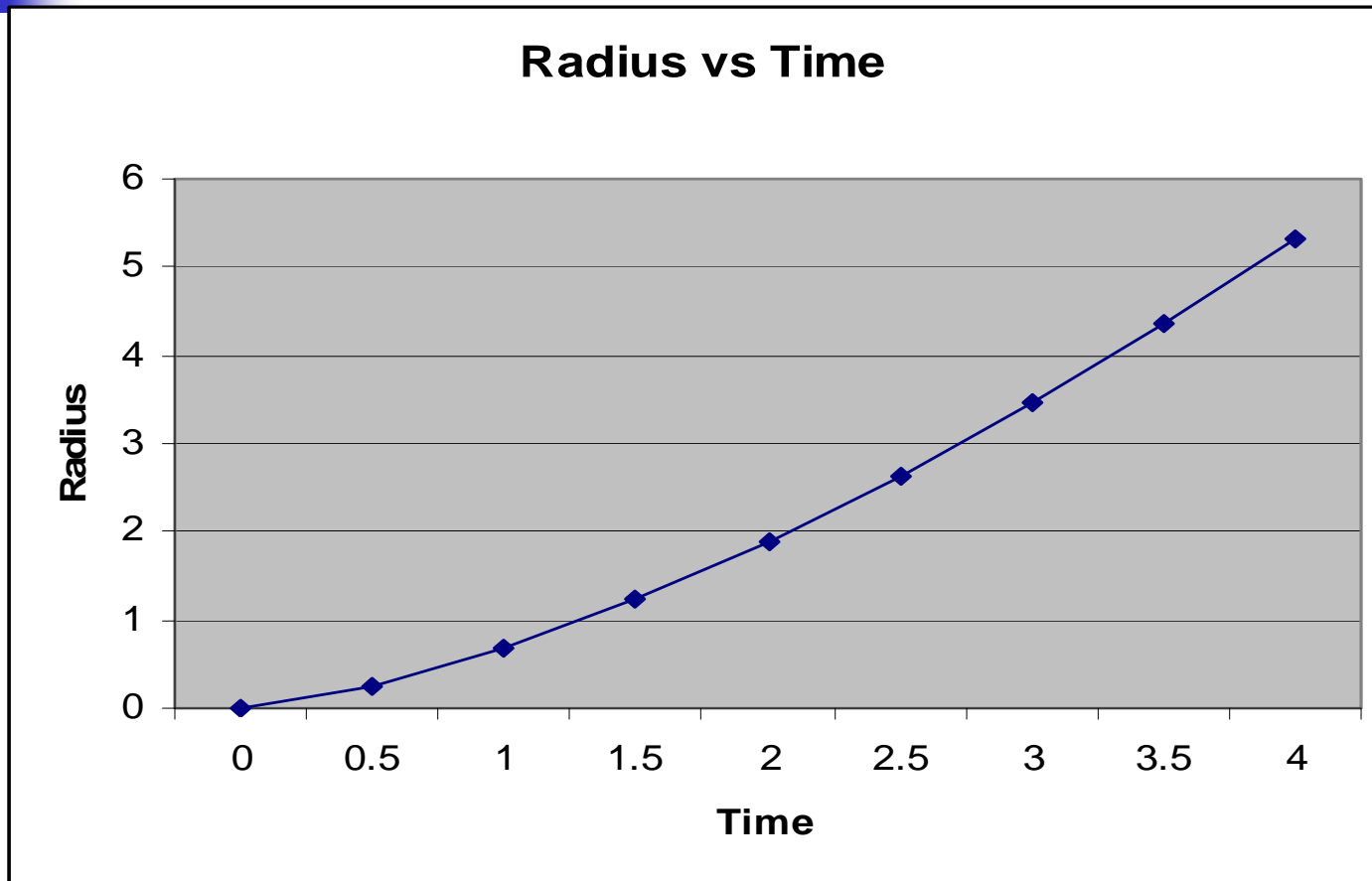
$$t_0 = 1.0, \quad R(t_0) = 0.667$$

$$t_1 = 1.5, \quad R(t_1) = 1.225$$

$$t_2 = 2.0, \quad R(t_2) = 1.886$$

$$t_3 = 2.5, \quad R(t_3) = 2.635$$

Example 2-Direct Fit Polynomials cont.





Example 2-Direct Fit Polynomials cont.

such that

$$R(1.0) = 0.667 = a_0 + a_1(1.0) + a_2(1.0)^2 + a_3(1.0)^3$$

$$R(1.5) = 1.225 = a_0 + a_1(1.5) + a_2(1.5)^2 + a_3(1.5)^3$$

$$R(2.0) = 1.886 = a_0 + a_1(2.0) + a_2(2.0)^2 + a_3(2.0)^3$$

$$R(2.5) = 2.635 = a_0 + a_1(2.5) + a_2(2.5)^2 + a_3(2.5)^3$$

Writing the four equations in matrix form, we have

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1.5 & 2.25 & 3.375 \\ 1 & 2 & 4 & 8 \\ 1 & 2.5 & 6.25 & 15.625 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 0.667 \\ 1.225 \\ 1.886 \\ 2.635 \end{bmatrix}$$



Example 2-Direct Fit Polynomials cont.

Solving the above four equations gives

$$a_0 = -0.080000$$

$$a_1 = 0.47100$$

$$a_2 = 0.29599$$

$$a_3 = -0.020000$$

Hence

$$\begin{aligned} R(t) &= a_0 + a_1t + a_2t^2 + a_3t^3 \\ &= -0.080000 + 0.47100t + 0.29599t^2 - 0.020000t^3, \quad 1 \leq t \leq 2.5 \end{aligned}$$

The derivative of radius at $t=2$ is given by

$$R'(2) = \left. \frac{d}{dt} E(t) \right|_{t=2}$$



Example 2-Direct Fit Polynomials cont.

Given that

$$R(t) = -0.080000 + 0.47100t + 0.29599t^2 - 0.020000t^3, \quad 1 \leq t \leq 2.5$$

$$\begin{aligned} R'(t) &= \frac{d}{dt} R(t) \\ &= \frac{d}{dt} (-0.080000 + 0.47100t + 0.29599t^2 - 0.020000t^3) \\ &= 0.47100 + 0.59180t - 0.060000t^2, \quad 1 \leq t \leq 2.5 \end{aligned}$$

$$R'(2) = 0.47100 + 0.59180(2) - 0.060000(2)^2$$

$$= 1.4146m / \text{sec}$$



Example 2-Direct Fit Polynomials cont.

(b) $Area = \pi R^2$

Time (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Area(m ²)	0	0.175	1.398	4.714	11.17	21.81	37.69	67.49	89.35

For the third order polynomial (also called cubic interpolation), we choose the radius given by $A(t) = a_0 + a_1t + a_2t^2 + a_3t^3$

Since we want to find the area at $t=2$, and we are using a third order polynomial, we need to choose the four points closest to $t=2$ and that also bracket $t=2$ to evaluate it.

The four points are $t_0=1.0$, $t_1=1.5$, $t_2=2.0$ and $t_3=2.5$.

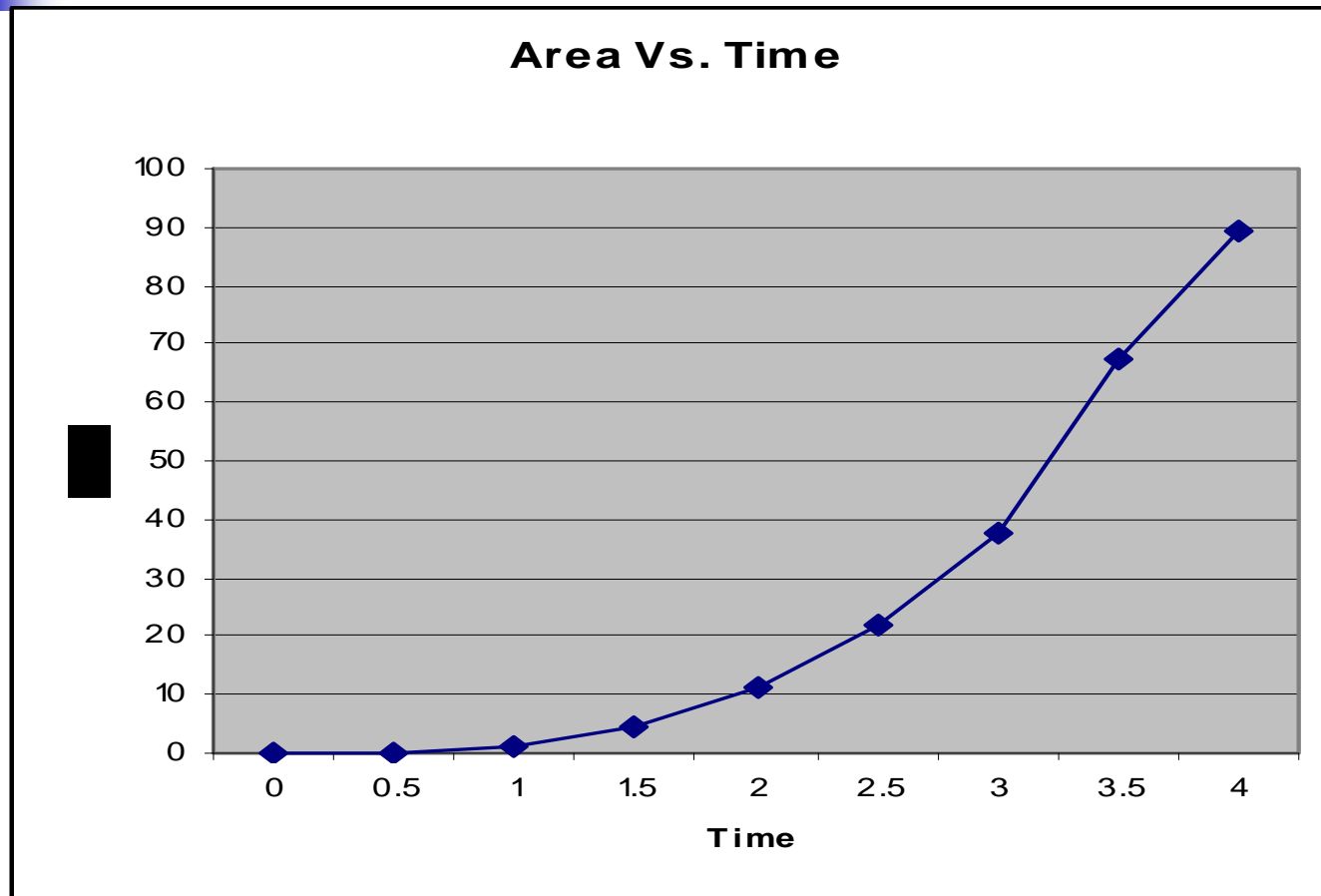
$$t_0 = 1.0, A(t_0) = 1.398$$

$$t_1 = 1.5, A(t_1) = 4.714$$

$$t_2 = 2.0, A(t_2) = 11.17$$

$$t_3 = 2.5, A(t_3) = 21.81$$

Example 2-Direct Fit Polynomials cont.





Example 2-fit Direct Polynomials cont.

such that

$$A(1.0) = 1.398 = a_0 + a_1(1.0) + a_2(1.0)^2 + a_3(1.0)^3$$

$$A(1.5) = 4.714 = a_0 + a_1(1.5) + a_2(1.5)^2 + a_3(1.5)^3$$

$$A(2.0) = 11.17 = a_0 + a_1(2.0) + a_2(2.0)^2 + a_3(2.0)^3$$

$$A(2.5) = 21.81 = a_0 + a_1(2.5) + a_2(2.5)^2 + a_3(2.5)^3$$

Writing the four equations in matrix form, we have

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1.5 & 2.25 & 3.375 \\ 1 & 2 & 4 & 8 \\ 1 & 2.5 & 6.25 & 15.625 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 1.398 \\ 4.714 \\ 11.17 \\ 21.81 \end{bmatrix}$$



Example 2- Direct Fit polynomials cont.

Solving the above four equations gives

$$a_0 = 0.0099$$

$$a_1 = -0.0199$$

$$a_2 = 0.016000$$

$$a_3 = 1.392$$

Hence

$$A(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$$

$$= 0.0099999 - 0.019999 t + 0.016000 t^2 + 1.3920 t^3, \quad 1 \leq t \leq 2.5$$

The derivative of radius at $t=2$ is given by

$$A'(2) = \left. \frac{d}{dt} E(t) \right|_{t=2}$$

Example 2- Direct Fit Polynomial cont

Given that

$$A(t) = 0.0099999 - 0.019999t + 0.016000t^2 + 1.3920t^3, \quad 1 \leq t \leq 2.5$$

$$\begin{aligned} A'(t) &= \frac{d}{dt} A(t) \\ &= \frac{d}{dt} (0.0099999 - 0.019999t + 0.016000t^2 + 1.3920t^3) \\ &= -0.019999 + 0.032000t + 4.176t^2, \quad 1 \leq t \leq 2.5 \end{aligned}$$

$$\begin{aligned} A'(2) &= -0.019999 + 0.032000(2) + 4.1760(2)^2 \\ &= 16.748 \quad m^2 / \text{sec} \end{aligned}$$



Lagrange Polynomial

In this method, given $(x_1, y_1), \dots, (x_n, y_n)$, one can fit a $(n-1)^{th}$ order Lagrangian polynomial given by

$$f_n(x) = \sum_{i=0}^n L_i(x) f(x_i)$$

where 'n' in $f_n(x)$ stands for the n^{th} order polynomial that approximates the function $y = f(x)$ given at $(n+1)$ data points as $(x_0, y_0), (x_1, y_1), \dots, (x_{n-1}, y_{n-1}), (x_n, y_n)$, and

$$L_i(x) = \prod_{\substack{j=0 \\ j \neq i}}^n \frac{x - x_j}{x_i - x_j}$$

$L_i(x)$ a weighting function that includes a product of $(n-1)$ terms with terms of $j = i$ omitted.



Lagrange Polynomial Cont.

Then to find the first derivative, one can differentiate $f_n(x)$ once, and so on for other derivatives.

For example, the second order Lagrange polynomial passing through

$(x_0, y_0), (x_1, y_1), (x_2, y_2)$ is

$$f_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$

Differentiating equation (2) gives



Lagrange Polynomial Cont.

$$f_2'(x) = \frac{2x - (x_1 + x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2x - (x_0 + x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2x - (x_0 + x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

Differentiating again would give the second derivative as

$$f_2''(x) = \frac{2}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$



Example 3

A new fuel for recreational boats being developed at the local university was tested at an are pond by a team of engineers. The interest is to document the environmental impact of the fuel – how quickly does the slick spreads? The table below shows the video camera record of the radius of the wave generated by a drop of the fuel that fell into the pond. Using the data

(a) Compute the rate at which the radius of the drop was changing at $t = 2$.

(b) Estimate the rate at which the area of the contaminant was spreading across the pond at $t = 2$.

Time (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Radius (m)	0	0.236	0.667	1.225	1.886	2.635	3.464	4.365	5.333

Use second order Lagrangian polynomial interpolation to solve the problem.



Example 3 Cont.

Solution:

$$(a) \quad R(t) = \left(\frac{t-t_1}{t_0-t_1} \right) \left(\frac{t-t_2}{t_0-t_2} \right) R(t_0) + \left(\frac{t-t_0}{t_1-t_0} \right) \left(\frac{t-t_2}{t_1-t_2} \right) R(t_1) + \left(\frac{t-t_0}{t_2-t_0} \right) \left(\frac{t-t_1}{t_2-t_1} \right) R(t_2)$$

$$R'(t) = \frac{2t - (t_1 + t_2)}{(t_0 - t_1)(t_0 - t_2)} R(t_0) + \frac{2t - (t_0 + t_2)}{(t_1 - t_0)(t_1 - t_2)} R(t_1)$$

$$+ \frac{2t - (t_0 + t_1)}{(t_2 - t_0)(t_2 - t_1)} R(t_2)$$

$$R'(2) = \frac{2(2) - (2.5 + 3)}{(1.5 - 2.5)(1.5 - 3)} (1.225)$$

$$+ \frac{2(2) - (1.5 + 3)}{(2.5 - 1.5)(2.5 - 3)} (2.63)$$

$$+ \frac{2(2) - (1.5 + 2.5)}{(3 - 1.5)(3 - 2.5)} (3.464)$$



Example 3 Cont.

$$= 1.4100 \text{ m/sec}$$

$$(b) \text{ Area} = \pi R^2$$

Time (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Area (m ²)	0	0.175	1.398	4.714	11.17	21.81	37.69	67.49	89.35

$$A(t) = \left(\frac{t-t_1}{t_0-t_1} \right) \left(\frac{t-t_2}{t_0-t_2} \right) A(t_0) + \left(\frac{t-t_0}{t_1-t_0} \right) \left(\frac{t-t_2}{t_1-t_2} \right) A(t_1) + \left(\frac{t-t_0}{t_2-t_0} \right) \left(\frac{t-t_1}{t_2-t_1} \right) A(t_2)$$

$$A'(t) = \frac{2t - (t_1 + t_2)}{(t_0 - t_1)(t_0 - t_2)} A(t_0) + \frac{2t - (t_0 + t_2)}{(t_1 - t_0)(t_1 - t_2)} A(t_1) + \frac{2t - (t_0 + t_1)}{(t_2 - t_0)(t_2 - t_1)} A(t_2)$$



Example 3 Cont.

$$A'(2) = \frac{2(2) - (2.5 + 3)}{(1.5 - 2.5)(1.5 - 3)}(4.714) + \frac{2(2) - (1.5 + 3)}{(2.5 - 1.5)(2.5 - 3)}(21.8) + \frac{2(2) - (1.5 + 2.5)}{(3 - 1.5)(3 - 2.5)}(37.69)$$
$$= 17.096 \text{ m}^2 / \text{sec}$$