Differentiation-Discrete Functions

Chemical Engineering Majors

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Transforming Numerical Methods Education for STEM Undergraduates

Differentiation –Discrete Functions

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Forward Difference Approximation

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

For a finite 'Δx'

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

Graphical Representation Of Forward Difference Approximation

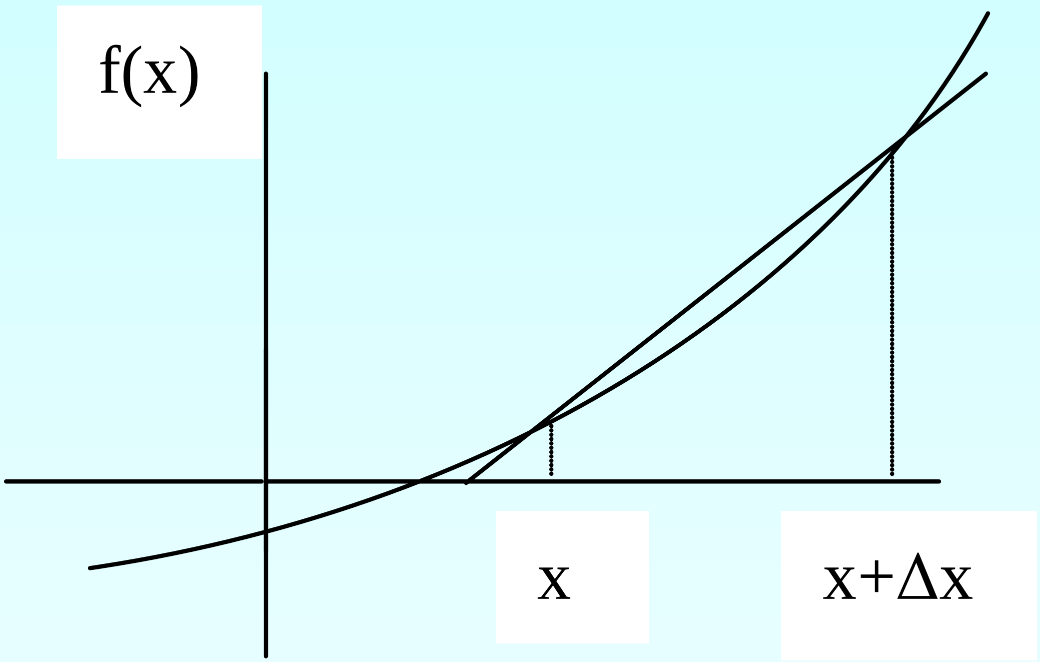

Figure 1 Graphical Representation of forward difference approximation of first derivative.

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? Table 1 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 $t = 2$ seconds.

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

Example 1 Cont.

Table 1 Radius as a function of time.

Time t (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Radius R (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) $$R'(t_i) \approx \frac{R(t_{i+1}) - R(t_i)}{\Delta t}$$

$$t_i = 2$$

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

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

$$= 2.5 - 2$$

$$= 0.5$$

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

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

$$\approx 1.498 \text{ m/s}$$

Example 1 Cont.

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

Time t (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Area A (m^2)	0	0.17497	1.3977	4.7144	11.175	21.813	37.697	59.857	89.350

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

$$t_i = 2$$

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

$$\begin{aligned} \Delta t &= t_{i+1} - t_i \\ &= 2.5 - 2 \\ &= 0.5 \end{aligned}$$

$$\begin{aligned} A'(10) &\approx \frac{A(2.5) - A(2)}{0.5} \\ &\approx \frac{21.813 - 11.175}{0.5} \\ &\approx 21.276 \text{m}^2/\text{s} \end{aligned}$$

Direct Fit Polynomials

In this method, given $'n+1'$ data points $(x_0, y_0), (x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$ one can fit a n^{th} order polynomial given by

$$P_n(x) = a_0 + a_1 x + \ldots\ldots + a_{n-1} x^{n-1} + a_n x^n$$

To find the first derivative,

$$P_n'(x) = \frac{dP_n(x)}{dx} = a_1 + 2a_2 x + \ldots\ldots + (n-1)a_{n-1} x^{n-2} + n a_n x^{n-1}$$

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

Table 2 Radius as a function of time.

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 calculations.

Example 2-Direct Fit Polynomials cont.

Solution

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

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

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 $t_0 = 1.0, t_1 = 1.5, t_2 = 2.0, \text{and } t_3 = 2.5.$

(Note: Choosing $t_0 = 1.5, t_1 = 2.0, t_2 = 2.5, \text{and } t_3 = 3.0$ is equally valid.)

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

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

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

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

Example 2-Direct Fit Polynomials cont.

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

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

$$= -0.080000 + 0.47100\,t + 0.29599\,t^2 - 0.020000\,t^3, \quad 1 \le t \le 2.5$$

Example 2-Direct Fit Polynomials cont.

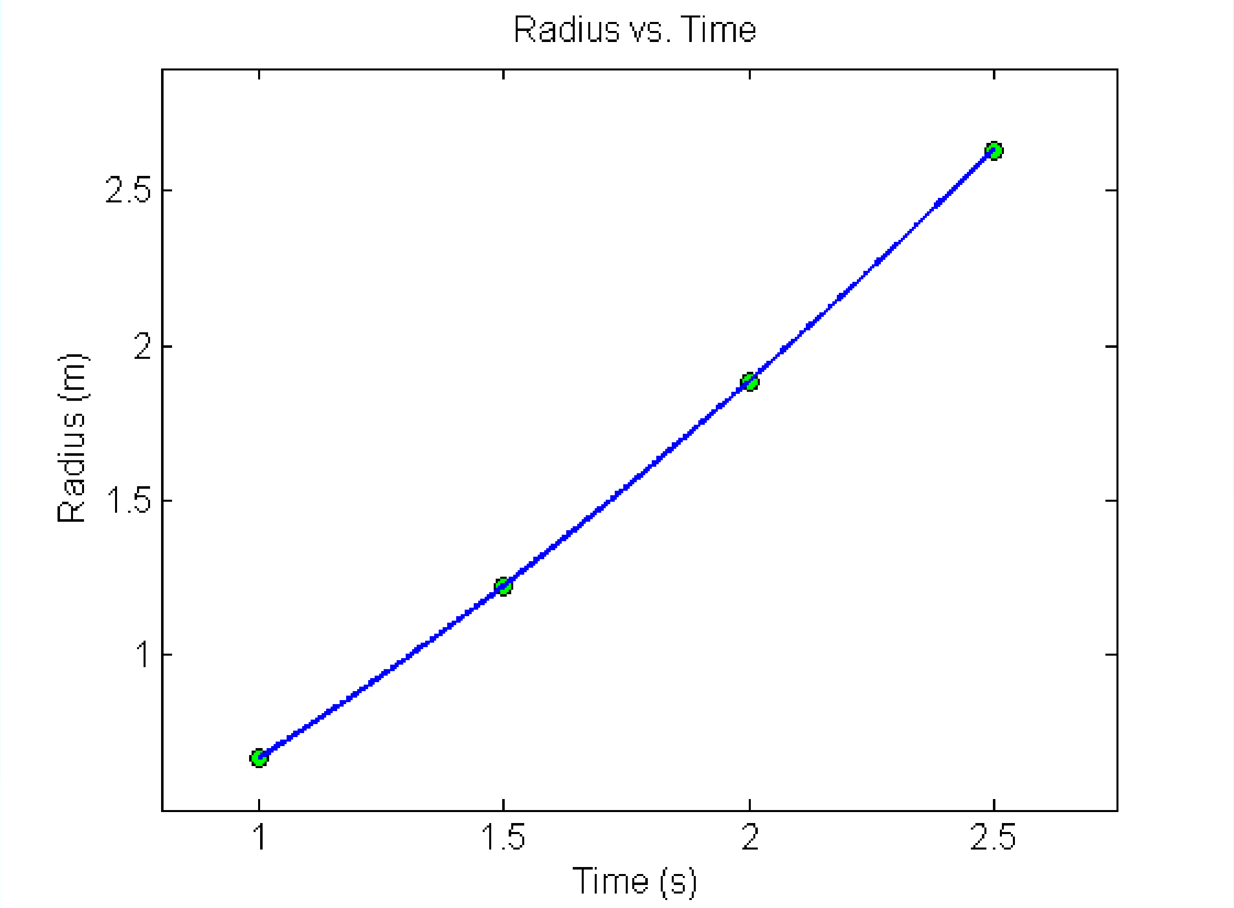

Figure 2 Graph of radius vs. time.

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Example 2-Direct Fit Polynomials cont.

The derivative of radius at t=2 is given by

$$R'(2)=\frac{d}{dt}R(t)\Big|_{t=2}$$

Given that

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

$$R'(t)=\frac{d}{dt}R(t)$$

$$=\frac{d}{dt}\left(-0.080000+0.47100t+0.29599t^2-0.020000t^3\right)$$

$$=0.47100+0.59180t-0.060000t^2,\quad 1\le t\le 2.5$$

$$R'(2)=0.47100+0.59180(2)\text{ - }0.060000(2)^2$$

$$=1.415\ \text{m/s}$$

Example 2-Direct Fit Polynomials cont.

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

Time t (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Area A (m^2)	0	0.17497	1.3977	4.7144	11.175	21.813	37.697	59.857	89.350

For the third order polynomial (also called cubic interpolation), we choose the area given by $A(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$

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 $t_3 = 2.5.$

(Note: Choosing $t_0 = 1.5, t_1 = 2.0, t_2 = 2.5,$ and $t_3 = 3.0$ is equally valid.)

$$t_o = 1.0, \quad A(t_o) = 1.3977$$

$$t_1 = 1.5, \quad A(t_1) = 4.7144$$

$$t_2 = 2.0, \quad A(t_2) = 11.175$$

$$t_3 = 2.5, \quad A(t_3) = 21.813$$

Example 2-fit Direct Ploynomials cont.

such that

$$A(1.0) = 1.3977 = a_0 + a_1(1.0) + a_2(1.0)^2 + a_3(1.0)^3$$

$$A(1.5) = 4.7144 = a_0 + a_1(1.5) + a_2(1.5)^2 + a_3(1.5)^3$$

$$A(2.0) = 11.175 = a_0 + a_1(2.0) + a_2(2.0)^2 + a_3(2.0)^3$$

$$A(2.5) = 21.813 = a_0 + a_1(2.5) + a_2(2.5)^2 + a_3(2.5)^3$$

Writing the four equations in matrix form, we have

$$\begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1.5 & 2.25 & 3.375 \\ 1 & 2 & 4 & 8 \\ 1 & 2.5 & 6.25 & 15.625 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 1.3977 \\ 4.7144 \\ 11.175 \\ 21.813 \end{bmatrix}$$

Example 2- Direct Fit polynomials cont.

Solving the above four equations gives

$$a_0 = 0.057900$$
$$a_1 = -0.12075$$
$$a_2 = 0.081468$$
$$a_3 = 1.3790$$

Hence

$$A(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$$
$$= 0.057900 - 0.12075t + 0.081468t^2 + 1.3790t^3, \quad 1 \le t \le 2.5$$

Example 2-Direct Fit Polynomials cont.

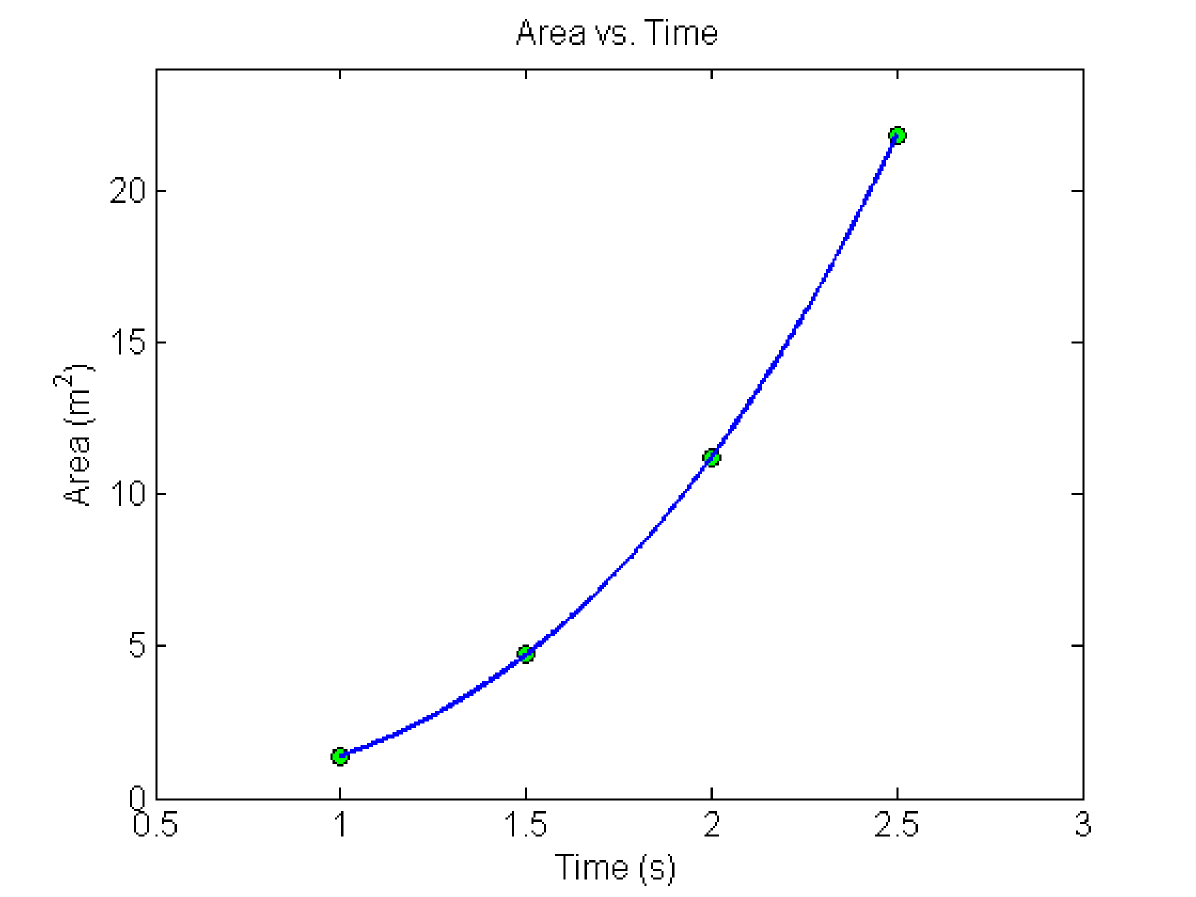

Figure 3 Graph of area vs. time.

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Example 2- Direct Fit Polynomial cont

The derivative of radius at t=2 is given by

Given that

$$A^{'}(2)=\frac{d}{dt}E(t)\Big|_{t=2}$$

$$A(t)=0.057900-0.12075t+0.081468t^{2}+1.3790t^{3}, \quad 1\le t\le 2.5$$

$$A^{'}(t) \;=\frac{d}{dt}A(t)$$

$$=\frac{d}{dt}\left(=0.057900-0.12075t+0.081468t^{2}+1.3790t^{3}\right)$$

$$=-0.12075+0.16294t+4.1371t^{2}, \quad 1\le t\le 2.5$$

$$A'(2)=-0.12075+0.16294(2)+4.1371(2)^{2}$$

$$=16.754\ \mathrm{m}^{2}/\mathrm{s}$$

Lagrange Polynomial

In this method, given $(x_1, y_1), \ldots, (x_n, y_n)$, 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 $(x_0, y_0), (x_1, y_1), \ldots\ldots, (x_{n-1}, y_{n-1}), (x_n, y_n)$, 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 spread? Table 3 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 $t = 2$.

Table 3 Radius as a function of time.

Time t (s)	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Radius R (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) For second order Lagrangian polynomial interpolation, we choose the radius given by

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

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

The three points are $t_0=1.5$, $t_1=2.0$, and $t_2=2.5$.

Differentiating the above equation gives

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

Hence,

$$R^{'}(2)=\frac{2(2)-(2.0+2.5)}{(1.5-2.0)(1.5-2.5)}(1.225)+\frac{2(2)-(1.5+2.5)}{(2.0-1.5)(2.0-2.5)}(1.886)+\frac{2(2)-(1.5+2.0)}{(2.5-1.5)(2.5-2.0)}(2.635)$$

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

Example 3 Cont.

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

Time $t\,(\mathrm{s})$	0	0.5	1.0	1.5	2.0	2.5	3.0	3.5	4.0
Area $A\,(\mathrm{m})$	0	0.17497	1.3977	4.7144	11.175	21.813	37.697	59.857	89.350

For second order Lagrangian polynomial interpolation, we choose the area given by

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

Example 3 Cont.

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

The three points are $t_0 = 1.5,\ t_1 = 2.0,$ and $t_2 = 2.5.$

Differentiating the above equation gives

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

Hence

$$A'(2) = \frac{2(2) - (2.0 + 2.5)}{(1.5 - 2.0)(1.5 - 2.5)}(4.7144) + \frac{2(2) - (1.5 + 2.5)}{(2.0 - 1.5)(2.0 - 2.5)}(11.175) + \frac{2(2) - (1.5 + 2.0)}{(2.5 - 1.5)(2.5 - 2.0)}(21.813)$$

$$= 17.099 \text{ m}^2/\text{s}$$

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/discrete_02dif.html

THE END

http://numericalmethods.eng.usf.edu