Differentiation –Discrete Functions

Computational Physics

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

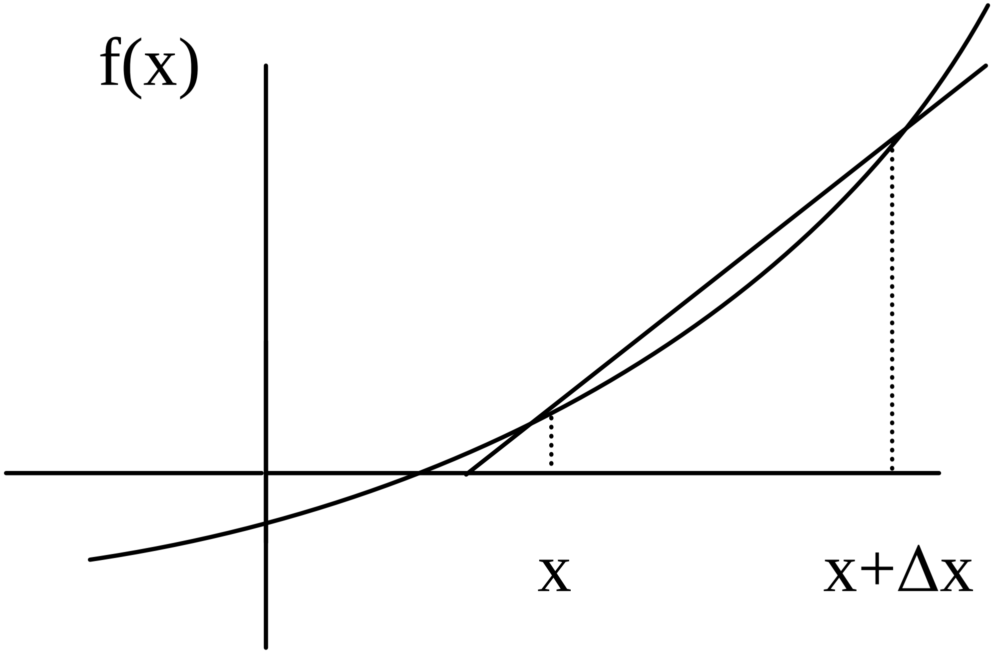

Figure 1 Graphical Representation of forward difference approximation of first derivative.

Example 1

The upward velocity of a rocket is given as a function of time in Table 1.

Table 1 Velocity as a function of time

t	**v(t)**
s	m/s
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

Using forward divided difference, find the acceleration of the rocket at $t = 16\ \text{s}$.

Example 1 Cont.

Solution

To find the acceleration at $t = 16\text{s}$, we need to choose the two values closest to $t = 16\text{s}$, that also bracket $t = 16\text{s}$ to evaluate it. The two points are $t = 15\text{s}$ and $t = 20\text{s}$.

$$a(t_i) \approx \frac{v(t_{i+1}) - v(t_i)}{\Delta t}$$

$$t_i = 15$$

$$t_{i+1} = 20$$

$$\begin{aligned}\Delta t &= t_{i+1} - t_i \\ &= 20 - 15 \\ &= 5\end{aligned}$$

Example 1 Cont.

$$a(16) \approx \frac{v(20) - v(15)}{5}$$

$$\approx \frac{517.35 - 362.78}{5}$$

$$\approx 30.914 \text{ m/s}^2$$

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,

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

Similarly other derivatives can be found.

Example 2-Direct Fit Polynomials

The upward velocity of a rocket is given as a function of time in Table 2.

Table 2 Velocity as a function of time

t	**v(t)**
s	m/s
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

Using the third order polynomial interpolant for velocity, find the acceleration of the rocket at $t = 16\ \text{s}$.

Example 2-Direct Fit Polynomials cont.

Solution

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

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

Since we want to find the velocity at $t = 16\ \mathrm{s}$, and we are using third order polynomial, we need to choose the four points closest to $t = 16\ \mathrm{s}$ and that also bracket $t = 16\ \mathrm{s}$ to evaluate it.

The four points are $t_o = 10, t_1 = 15,\ t_2 = 20,\ \text{and}\ \ t_3 = 22.5.$

$$t_o = 10,\ \ v(t_o) = 227.04$$

$$t_1 = 15,\ \ v(t_1) = 362.78$$

$$t_2 = 20,\ \ v(t_2) = 517.35$$

$$t_3 = 22.5,\ \ v(t_3) = 602.97$$

Example 2-Direct Fit Polynomials cont.

such that

$$v(10) = 227.04 = a_0 + a_1(10) + a_2(10)^2 + a_3(10)^3$$

$$v(15) = 362.78 = a_0 + a_1(15) + a_2(15)^2 + a_3(15)^3$$

$$v(20) = 517.35 = a_0 + a_1(20) + a_2(20)^2 + a_3(20)^3$$

$$v(22.5) = 602.97 = a_0 + a_1(22.5) + a_2(22.5)^2 + a_3(22.5)^3$$

Writing the four equations in matrix form, we have

$$\begin{bmatrix} 1 & 10 & 100 & 1000 \\ 1 & 15 & 225 & 3375 \\ 1 & 20 & 400 & 8000 \\ 1 & 22.5 & 506.25 & 11391 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 227.04 \\ 362.78 \\ 517.35 \\ 602.97 \end{bmatrix}$$

Example 2-Direct Fit Polynomials cont.

Solving the above four equations gives

$$a_0 = -4.3810$$

$$a_1 = 21.289$$

$$a_2 = 0.13065$$

$$a_3 = 0.0054606$$

Hence

$$\begin{aligned} v(t) &= a_0 + a_1 t + a_2 t^2 + a_3 t^3 \\ &= -4.3810 + 21.289t + 0.13065t^2 + 0.0054606t^3, \quad 10 \le t \le 22.5 \end{aligned}$$

Example 2-Direct Fit Polynomials cont.

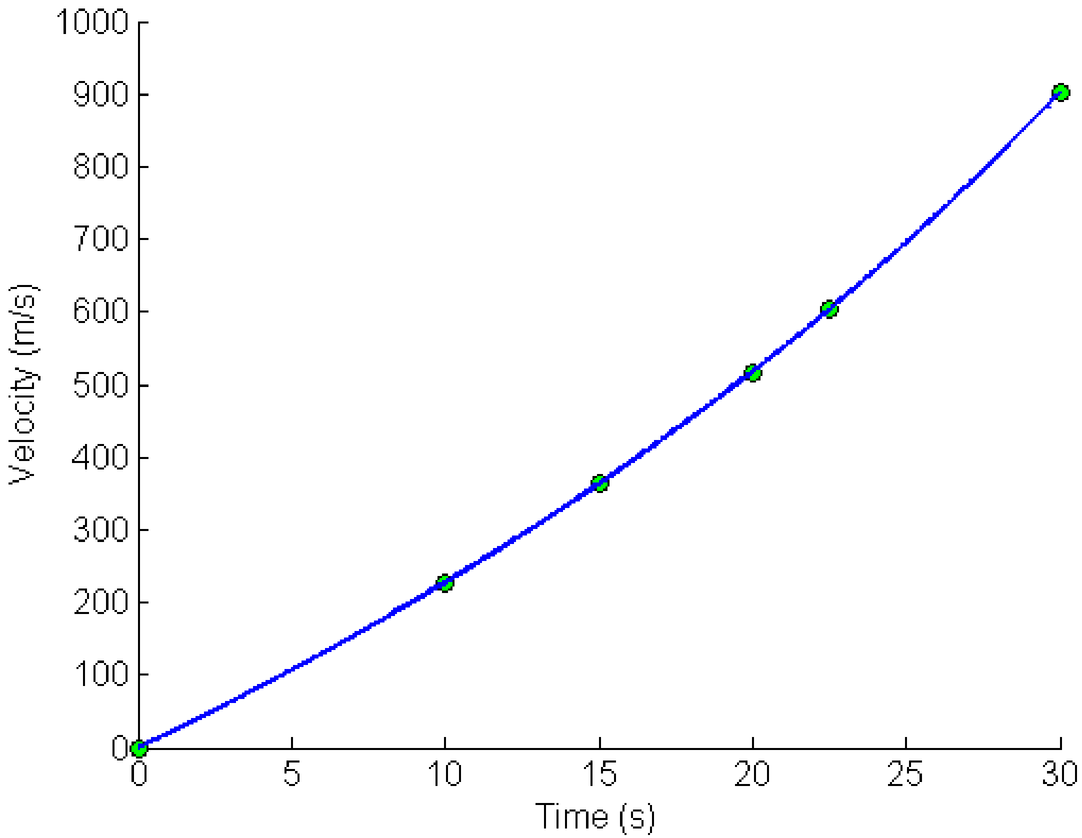

Figure 1 Graph of upward velocity of the rocket vs. time.

,

Example 2-Direct Fit Polynomials cont.

The acceleration at t=16 is given by

$$a(16) = \frac{d}{dt} v(t)\Big|_{t=16}$$

Given that

$$v(t) = -4.3810 + 21.289t + 0.13065t^2 + 0.0054606t^3, 10 \le t \le 22.5$$

$$a(t) \quad = \frac{d}{dt} v(t)$$

$$= \frac{d}{dt}\left(-4.3810 + 21.289t + 0.13065t^2 + 0.0054606t^3\right)$$

$$= 21.289 + 0.26130t + 0.016382t^2, \quad 10 \le t \le 22.5$$

$$a(16) = 21.289 + 0.26130(16) + 0.016382(16)^2$$

$$= 29.664 \text{m/s}^2$$

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

The upward velocity of a rocket is given as a function of time in Table 3.

Table 3 Velocity as a function of time

t	**v(t)**
s	m/s
0	0
10	227.04
15	362.78
20	517.35
22.5	602.97
30	901.67

Determine the value of the acceleration at $t = 16\ \text{s}$ using the second order Lagrangian polynomial interpolation for velocity.

Example 3 Cont.

Solution

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

$$a(t)=\frac{2t-(t_1+t_2)}{(t_0-t_1)(t_0-t_2)}v(t_0)+\frac{2t-(t_0+t_2)}{(t_1-t_0)(t_1-t_2)}v(t_1)+\frac{2t-(t_0+t_1)}{(t_2-t_0)(t_2-t_1)}v(t_2)$$

$$a(16)=\frac{2(16)-(15+20)}{(10-15)(10-20)}(227.04)+\frac{2(16)-(10+20)}{(15-10)(15-20)}(362.78)+\frac{2(16)-(10+15)}{(20-10)(20-15)}(517.35)$$

$$=-0.06(227.04)-0.08(362.78)+0.14(517.35)$$

$$=29.784\text{m/s}^2$$

THE END