

Differentiation – Continuous Functions

Computational Physics

Forward Difference Approximation

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

For a finite ' Δx '

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

Graphical Representation Of Forward Difference Approximation

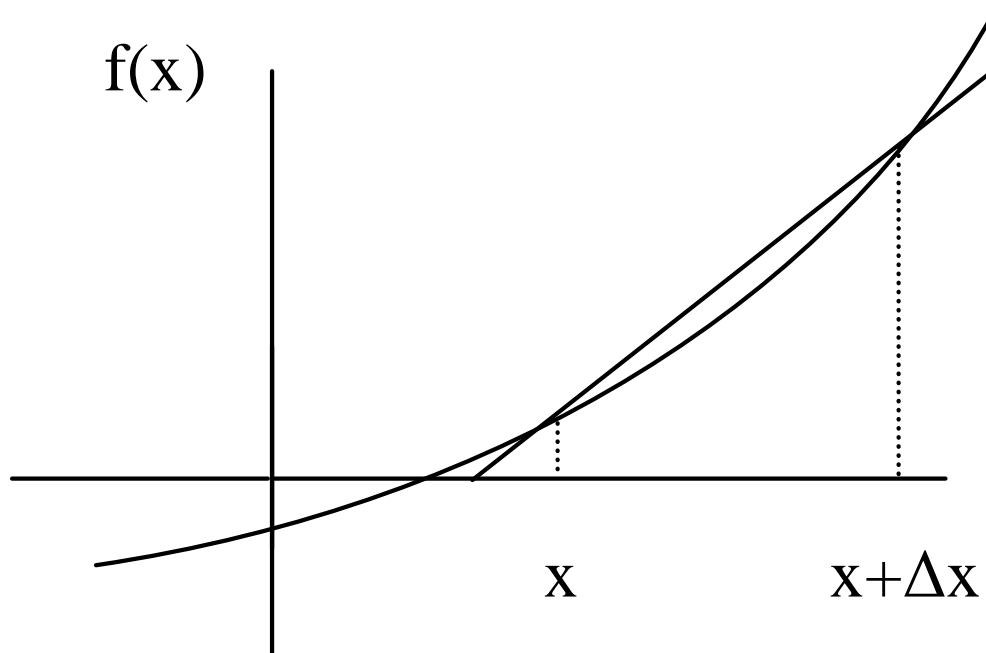


Figure 1 Graphical Representation of forward difference approximation of first derivative.

Example 1

The velocity of a rocket is given by

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t, 0 \leq t \leq 30$$

where ' v ' is given in m/s and ' t ' is given in seconds.

- Use forward difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2s$.
- Find the exact value of the acceleration of the rocket.
- Calculate the absolute relative true error for part (b).

Example 1 Cont.

Solution

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

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ &= 16 + 2 \\ &= 18 \end{aligned}$$

$$a(16) \approx \frac{v(18) - v(16)}{2}$$

Example 1 Cont.

$$\begin{aligned}v(18) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)} \right] - 9.8(18) \\ &= 453.02 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(16) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)} \right] - 9.8(16) \\ &= 392.07 \text{m/s}\end{aligned}$$

Hence

$$a(16) \approx \frac{v(18) - v(16)}{2}$$

Example 1 Cont.

$$\approx \frac{453.02 - 392.07}{2}$$
$$\approx 30.474 \text{m/s}^2$$

b) The exact value of $a(16)$ can be calculated by differentiating

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t$$

as

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

Example 1 Cont.

Knowing that

$$\frac{d}{dt}[\ln(t)] = \frac{1}{t} \quad \text{and} \quad \frac{d}{dt}\left[\frac{1}{t}\right] = -\frac{1}{t^2}$$

$$\begin{aligned} a(t) &= 2000 \left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4} \right) \frac{d}{dt} \left(\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right) - 9.8 \\ &= 2000 \left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4} \right) (-1) \left(\frac{14 \times 10^4}{(14 \times 10^4 - 2100t)^2} \right) (-2100) - 9.8 \\ &= \frac{-4040 - 29.4t}{-200 + 3t} \end{aligned}$$

Example 1 Cont.

$$a(16) = \frac{-4040 - 29.4(16)}{-200 + 3(16)}$$
$$= 29.674 \text{m/s}^2$$

The absolute relative true error is

$$|\epsilon_t| = \left| \frac{\text{True Value} - \text{Approximate Value}}{\text{True Value}} \right| \times 100$$
$$= \left| \frac{29.674 - 30.474}{29.674} \right| \times 100$$
$$= 2.6967\%$$

Backward Difference Approximation of the First Derivative

We know

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

For a finite ' Δx ',

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

If ' Δx ' is chosen as a negative number,

$$\begin{aligned} f'(x) &\approx \frac{f(x - \Delta x) - f(x)}{-\Delta x} \\ &= \frac{f(x) - f(x - \Delta x)}{\Delta x} \end{aligned}$$

Backward Difference Approximation of the First Derivative Cont.

This is a backward difference approximation as you are taking a point backward from x . To find the value of $f'(x)$ at $x = x_i$, we may choose another point ' Δx ' behind as $x = x_{i-1}$. This gives

$$\begin{aligned} f'(x_i) &\approx \frac{f(x_i) - f(x_{i-1})}{\Delta x} \\ &= \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \end{aligned}$$

where

$$\Delta x = x_i - x_{i-1}$$

Backward Difference Approximation of the First Derivative Cont.

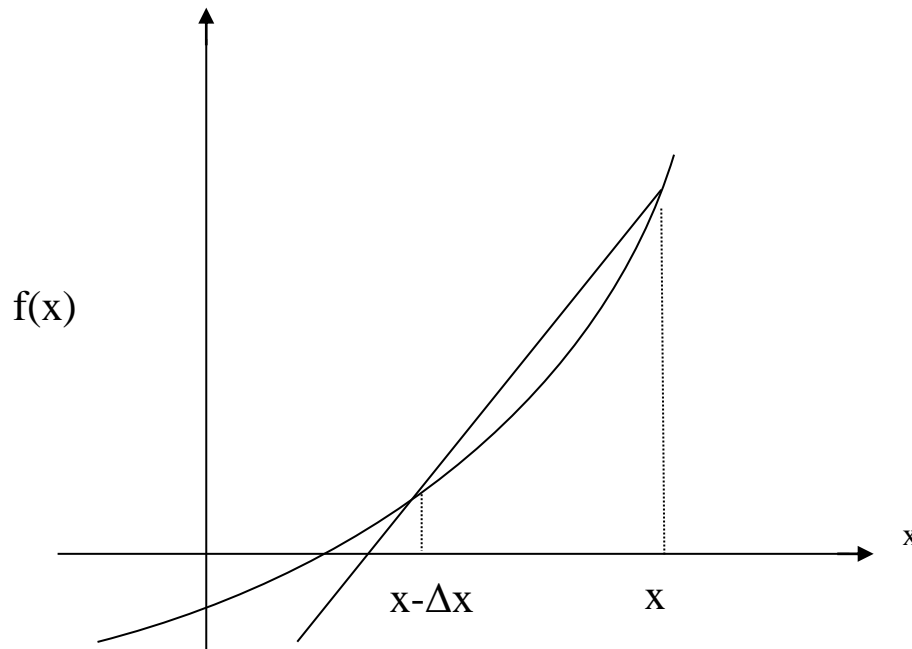


Figure 2 Graphical Representation of backward difference approximation of first derivative

Example 2

The velocity of a rocket is given by

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t, 0 \leq t \leq 30$$

where ' v ' is given in m/s and ' t ' is given in seconds.

- Use backward difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16\text{ s}$. Use a step size of $\Delta t = 2\text{ s}$.
- Find the absolute relative true error for part (a).

Example 2 Cont.

Solution

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

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i-1} &= t_i - \Delta t \\ &= 16 - 2 \\ &= 14 \end{aligned}$$

$$a(16) \approx \frac{v(16) - v(14)}{2}$$

Example 2 Cont.

$$\begin{aligned}v(16) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)} \right] - 9.8(16) \\ &= 392.07 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(14) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(14)} \right] - 9.8(14) \\ &= 334.24 \text{m/s}\end{aligned}$$

$$\begin{aligned}a(16) &\approx \frac{v(16) - v(14)}{2} \\ &= \frac{392.07 - 334.24}{2} \\ &\approx 28.915 \text{m/s}^2\end{aligned}$$

Example 2 Cont.

The exact value of the acceleration at $t = 16\text{ s}$ from Example 1 is

$$a(16) = 29.674\text{ m/s}^2$$

The absolute relative true error is

$$|\epsilon_t| = \left| \frac{29.674 - 28.915}{29.674} \right| \times 100$$

$$= 2.5584\%$$

Derive the forward difference approximation from Taylor series

Taylor's theorem says that if you know the value of a function ' f ' at a point x_i and all its derivatives at that point, provided the derivatives are continuous between x_i and x_{i+1} , then

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 + \dots$$

Substituting for convenience $\Delta x = x_{i+1} - x_i$

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \dots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} - \frac{f''(x_i)}{2!}(\Delta x) + \dots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{\Delta x} + O(\Delta x)$$

Derive the forward difference approximation from Taylor series Cont.

The $(O\Delta x)$ term shows that the error in the approximation is of the order of (Δx) . Can you now derive from Taylor series the formula for backward divided difference approximation of the first derivative?

As shown above, both forward and backward divided difference approximation of the first derivative are accurate on the order of $(O\Delta x)$.

Can we get better approximations? Yes, another method to approximate the first derivative is called the **Central difference approximation of the first derivative.**

Derive the forward difference approximation from Taylor series Cont.

From Taylor series

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \dots$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \dots$$

Subtracting equation (2) from equation (1)

$$f(x_{i+1}) - f(x_{i-1}) = f'(x_i)(2\Delta x) + \frac{2f'''(x_i)}{3!}(\Delta x)^3 + \dots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} - \frac{f'''(x_i)}{3!}(\Delta x)^2 + \dots$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2\Delta x} + O(\Delta x)^2$$

Central Divided Difference

Hence showing that we have obtained a more accurate formula as the error is of the order of $O(\Delta x)^2$.

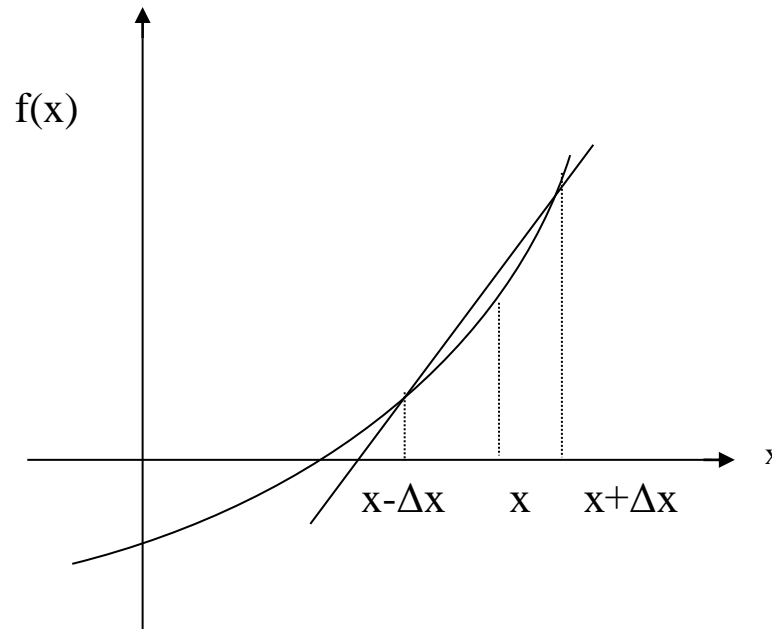


Figure 3 Graphical Representation of central difference approximation of first derivative

Example 3

The velocity of a rocket is given by

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t, 0 \leq t \leq 30$$

where ' v ' is given in m/s and ' t ' is given in seconds.

- (a) Use central divided difference approximation of the first derivative of $v(t)$ to calculate the acceleration at $t = 16s$. Use a step size of $\Delta t = 2s$.
- (b) Find the absolute relative true error for part (a).

Example 3 cont.

Solution

$$a(t_i) \approx \frac{v(t_{i+1}) - v(t_{i-1}))}{2\Delta t}$$

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ &= 16 + 2 \\ &= 18 \end{aligned}$$

$$\begin{aligned} t_{i-1} &= t_i - \Delta t \\ &= 16 - 2 \\ &= 14 \end{aligned}$$

$$\begin{aligned} a(16) &\approx \frac{v(18) - v(14)}{2(2)} \\ &\approx \frac{v(18) - v(14)}{4} \end{aligned}$$

Example 3 cont.

$$\begin{aligned}v(18) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)} \right] - 9.8(18) \\ &= 453.02 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(14) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(14)} \right] - 9.8(14) \\ &= 334.24 \text{m/s}\end{aligned}$$

$$\begin{aligned}a(16) &\approx \frac{v(18) - v(14)}{4} \\ &\approx \frac{453.02 - 334.24}{4} \\ &\approx 29.694 \text{m/s}^2\end{aligned}$$

Example 3 cont.

The exact value of the acceleration at $t = 16\text{ s}$ from Example 1 is

$$a(16) = 29.674\text{ m/s}^2$$

The absolute relative true error is

$$\begin{aligned} |\epsilon_t| &= \left| \frac{29.674 - 29.694}{29.674} \right| \times 100 \\ &= 0.069157\% \end{aligned}$$

Comparison of FDD, BDD, CDD

The results from the three difference approximations are given in Table 1.

Table 1 Summary of $a(16)$ using different divided difference approximations

Type of Difference Approximation	$a(16)$ (m/s^2)	$ \epsilon_t \%$
Forward	30.475	2.6967
Backward	28.915	2.5584
Central	29.695	0.069157

Finding the value of the derivative within a prespecified tolerance

In real life, one would not know the exact value of the derivative – so how would one know how accurately they have found the value of the derivative. A simple way would be to start with a step size and keep on halving the step size and keep on halving the step size until the absolute relative approximate error is within a pre-specified tolerance.

Take the example of finding $v'(t)$ for

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t$$

at $t = 16$ using the backward divided difference scheme.

Finding the value of the derivative within a prespecified tolerance Cont.

Given in Table 2 are the values obtained using the backward difference approximation method and the corresponding absolute relative approximate errors.

Table 2 First derivative approximations and relative errors for different Δt values of backward difference scheme

Δt	$v'(t)$	$ \epsilon_a \%$
2	28.915	
1	29.289	1.2792
0.5	29.480	0.64787
0.25	29.577	0.32604
0.125	29.625	0.16355

Finding the value of the derivative within a prespecified tolerance Cont.

From the above table, one can see that the absolute relative approximate error decreases as the step size is reduced. At $\Delta t = 0.125$ the absolute relative approximate error is 0.16355%, meaning that at least 2 significant digits are correct in the answer.

Finite Difference Approximation of Higher Derivatives

One can use Taylor series to approximate a higher order derivative.

For example, to approximate $f''(x)$, the Taylor series for

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2\Delta x) + \frac{f''(x_i)}{2!}(2\Delta x)^2 + \frac{f'''(x_i)}{3!}(2\Delta x)^3 + \dots$$

where

$$x_{i+2} = x_i + 2\Delta x$$

$$f(x_{i+1}) = f(x_i) + f'(x_i)(\Delta x) + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 \dots$$

where

$$x_{i-1} = x_i - \Delta x$$

Finite Difference Approximation of Higher Derivatives Cont.

Subtracting 2 times equation (4) from equation (3) gives

$$f(x_{i+2}) - 2f(x_{i+1}) = -f(x_i) + f''(x_i)(\Delta x)^2 + f'''(x_i)(\Delta x)^3 \dots$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2} - f'''(x_i)(\Delta x) + \dots$$

$$f''(x_i) \cong \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{(\Delta x)^2} + O(\Delta x) \quad (5)$$

Example 4

The velocity of a rocket is given by

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t, 0 \leq t \leq 30$$

Use forward difference approximation of the second derivative $v''(t)$ of to calculate the jerk at $t = 16s$. Use a step size of $\Delta t = 2s$.

Example 4 Cont.

Solution

$$j(t_i) \approx \frac{v(t_{i+2}) - 2v(t_{i+1}) + v(t_i)}{(\Delta t)^2}$$

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ &= 16 + 2 \\ &= 18 \end{aligned}$$

$$\begin{aligned} t_{i+2} &= t_i + 2(\Delta t) \\ &= 16 + 2(2) \\ &= 20 \end{aligned}$$

$$j(16) \approx \frac{v(20) - 2v(18) + v(16)}{(2)^2}$$

Example 4 Cont.

$$\begin{aligned}v(20) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(20)} \right] - 9.8(20) \\ &= 517.35 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(18) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)} \right] - 9.8(18) \\ &= 453.02 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(16) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)} \right] - 9.8(16) \\ &= 392.07 \text{m/s}\end{aligned}$$

Example 4 Cont.

$$j(16) \approx \frac{517.35 - 2(453.02) + 392.07}{4}$$
$$\approx 0.84515 \text{m/s}^3$$

The exact value of $j(16)$ can be calculated by differentiating

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t$$

twice as

$$a(t) = \frac{d}{dt} [v(t)] \quad \text{and} \quad j(t) = \frac{d}{dt} [a(t)]$$

Example 4 Cont.

Knowing that

$$\frac{d}{dt} [\ln(t)] = \frac{1}{t} \quad \text{and} \quad \frac{d}{dt} \left[\frac{1}{t} \right] = -\frac{1}{t^2}$$

$$\begin{aligned} a(t) &= 2000 \left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4} \right) \frac{d}{dt} \left(\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right) - 9.8 \\ &= 2000 \left(\frac{14 \times 10^4 - 2100t}{14 \times 10^4} \right) (-1) \left(\frac{14 \times 10^4}{(14 \times 10^4 - 2100t)^2} \right) (-2100) - 9.8 \\ &= \frac{-4040 - 29.4t}{-200 + 3t} \end{aligned}$$

Example 4 Cont.

Similarly it can be shown that

$$\begin{aligned}j(t) &= \frac{d}{dt}[a(t)] \\ &= \frac{18000}{(-200 + 3t)^2}\end{aligned}$$

$$\begin{aligned}j(16) &= \frac{18000}{[-200 + 3(16)]^2} \\ &= 0.77909 \text{m/s}^3\end{aligned}$$

The absolute relative true error is

$$\begin{aligned}|\epsilon_t| &= \left| \frac{0.77909 - 0.84515}{0.77909} \right| \times 100 \\ &= 8.4797 \%\end{aligned}$$

Higher order accuracy of higher order derivatives

The formula given by equation (5) is a forward difference approximation of the second derivative and has the error of the order of (Δx) . Can we get a formula that has a better accuracy? We can get the central difference approximation of the second derivative.

The Taylor series for

$$f(x_{i+1}) = f(x_i) + f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 + \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f^{(4)}(x_i)}{4!}(\Delta x)^4 \dots \quad (6)$$

where

$$x_{i+1} = x_i + \Delta x$$

Higher order accuracy of higher order derivatives Cont.

$$f(x_{i-1}) = f(x_i) - f'(x_i)\Delta x + \frac{f''(x_i)}{2!}(\Delta x)^2 - \frac{f'''(x_i)}{3!}(\Delta x)^3 + \frac{f^{(4)}(x_i)}{4!}(\Delta x)^4 \dots \quad (7)$$

where

$$x_{i-1} = x_i - \Delta x$$

Adding equations (6) and (7), gives

$$f(x_{i+1}) + f(x_{i-1}) = 2f(x_i) + f''(x_i)(\Delta x)^2 + f'''(x_i)\frac{(\Delta x)^4}{12}$$

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{(\Delta x)^2} - \frac{f'''(x_i)(\Delta x)^2}{12}$$

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1}))}{(\Delta x)^2} + O(\Delta x)^2$$

Example 5

The velocity of a rocket is given by

$$v(t) = 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100t} \right] - 9.8t, 0 \leq t \leq 30$$

Use central difference approximation of second derivative of $v(t)$ to calculate the jerk at $t = 16s$. Use a step size of $\Delta t = 2s$.

Example 5 Cont.

Solution

$$a(t_i) \approx \frac{v(t_{i+1}) - 2v(t_i) + v(t_{i-1}))}{(\Delta t)^2}$$

$$t_i = 16$$

$$\Delta t = 2$$

$$\begin{aligned} t_{i+1} &= t_i + \Delta t \\ &= 16 + 2 \\ &= 18 \end{aligned}$$

$$\begin{aligned} t_{i-1} &= t_i - \Delta t \\ &= 16 - 2 \\ &= 14 \end{aligned}$$

$$j(16) \approx \frac{v(18) - 2v(16) + v(14)}{(2)^2}$$

Example 5 Cont.

$$\begin{aligned}v(18) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(18)} \right] - 9.8(18) \\ &= 453.02 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(16) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(16)} \right] - 9.8(16) \\ &= 392.07 \text{m/s}\end{aligned}$$

$$\begin{aligned}v(14) &= 2000 \ln \left[\frac{14 \times 10^4}{14 \times 10^4 - 2100(14)} \right] - 9.8(14) \\ &= 334.24 \text{m/s}\end{aligned}$$

Example 5 Cont.

$$\begin{aligned}j(16) &\approx \frac{v(18) - 2v(16) + v(14)}{(2)^2} \\ &\approx \frac{453.02 - 2(392.07) + 334.24}{4} \\ &\approx 0.77969 \text{m/s}^3\end{aligned}$$

The absolute relative true error is

$$\begin{aligned}|\epsilon_t| &= \left| \frac{0.77908 - 0.78}{0.77908} \right| \times 100 \\ &= 0.077992\%\end{aligned}$$

THE END

Computational Physics