Numerical Differentiation

- Calculus is the mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of engineering.
- Standing in the heart of calculus are the mathematical concepts of *differentiation* and *integration*:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

$$I = \int_a^b f(x)\,dx$$

Noncomputer Methods for Differentiation and Integration

- The function to be differentiated or integrated will typically be in one of the following three forms:
  - A simple continuous function such as polynomial, an exponential, or a trigonometric function.
  - A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
  - A tabulated function where values of x and f(x) are given at a number of discrete points, as is often the case with experimental or field data.

Forward Difference Approximation

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

For a finite $'\Delta x'$

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

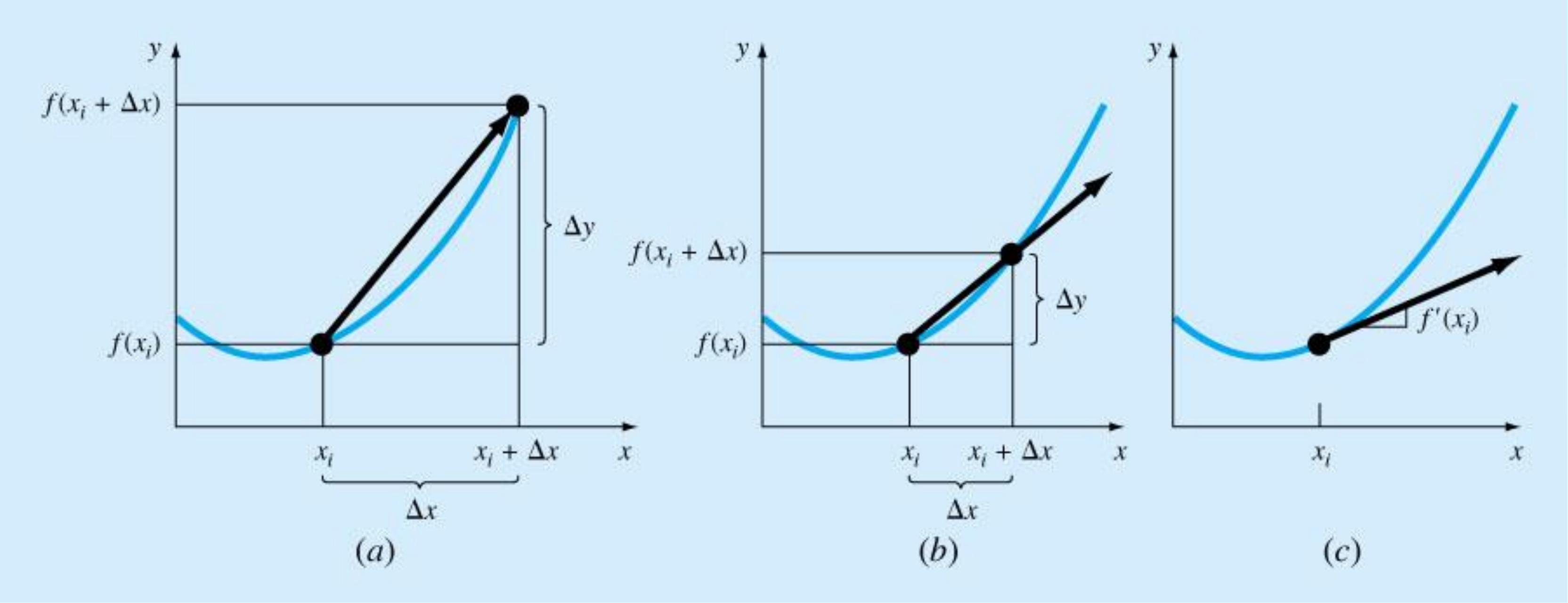
For the discrete case

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

Absolute relative true error

$$|\in_t| = \left| \frac{\text{True Value - Approximat e Value}}{\text{True Value}} \right| x100$$

Graphical Representation Of Forward Difference Approximation



Example 1 (Discrete)

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.

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

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

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

Example 2 (Continuous Case)

The velocity of a rocket is given by

$$v(t) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30$$

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

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

Example 2 Cont.

Solution

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

$$t_i = 16$$

$$\Delta t = 2$$

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

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

Example 2 Cont.

$$\nu(18) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(18)}\right] - 9.8(18)$$

$$= 453.02\,\text{m/s}$$

$$\nu(16) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07\,\text{m/s}$$

Hence

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

Example 2 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

$$v(t) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t$$

as

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

Example 2 Cont.

Analytical Solution (TRUE or Symbolic): Knowing that

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

$$a(t)=2000\left(\frac{14\times10^4-2100t}{14\times10^4}\right)\frac{d}{dt}\left(\frac{14\times10^4}{14\times10^4-2100t}\right)-9.8$$

$$=2000\left(\frac{14\times10^4-2100t}{14\times10^4}\right)(-1)\left(\frac{14\times10^4}{\left(14\times10^4-2100t\right)^2}\right)(-2100)-9.8$$

$$=\frac{-4040-29.4t}{-200+3t}$$

Example 2 Cont.

$$a(16) = \frac{-4040 - 29.4(16)}{-200 + 3(16)}$$

$$= 29.674 \text{ m/s}^2$$

The absolute relative true error is

$$\left|\in_t\right| = \left|\frac{\text{True Value - Approximat e Value}}{\text{True Value}}\right| x100$$

$$= \left|\frac{29.674 - 30.474}{29.674}\right| x100$$

$$= 2.6967\,\%$$

Backward Difference Approximation

We know

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

For a finite $'\Delta x'$,

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

If $'\Delta x'$ is chosen as a negative number,

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

$$= \frac{f(x) - f(x-\Delta x)}{\Delta x}$$

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

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

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

where

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

Backward Difference Approximation of the First Derivative Cont.

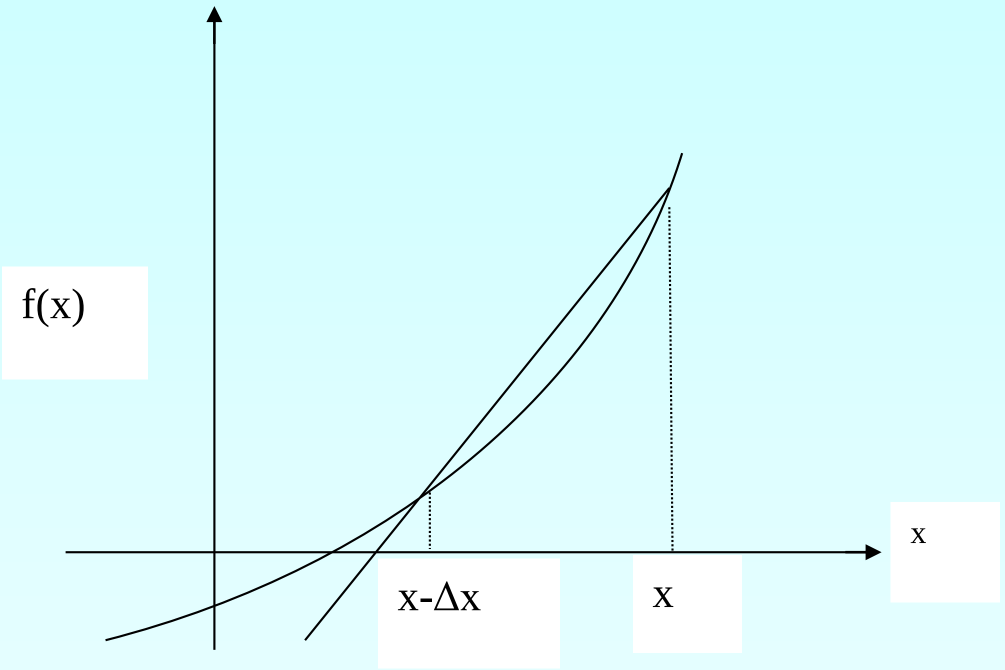


Figure 2 Graphical Representation of backward difference approximation of first derivative

Example 3

The velocity of a rocket is given by

$$v(t) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30$$

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

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

Example 3 Cont.

Solution

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

$$t_i = 16$$

$$\Delta t = 2$$

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

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

Example 3 Cont.

$$\nu(16) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(16)}\right] - 9.8(16)$$

$$= 392.07\,\text{m/s}$$

$$\nu(14) = 2000\ln\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14)$$

$$= 334.24\,\text{m/s}$$

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

$$= \frac{392.07 - 334.24}{2}$$

$$\approx 28.915\,\text{m/s}^2$$

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

$$|\in_t| = \left|\frac{29.674 - 28.915}{29.674}\right| x100$$

$$= 2.5584\%$$

Central Divided Difference

Hence showing that we have obtained a more accurate formula as the error is of the order of $0(\Delta x)^2$.

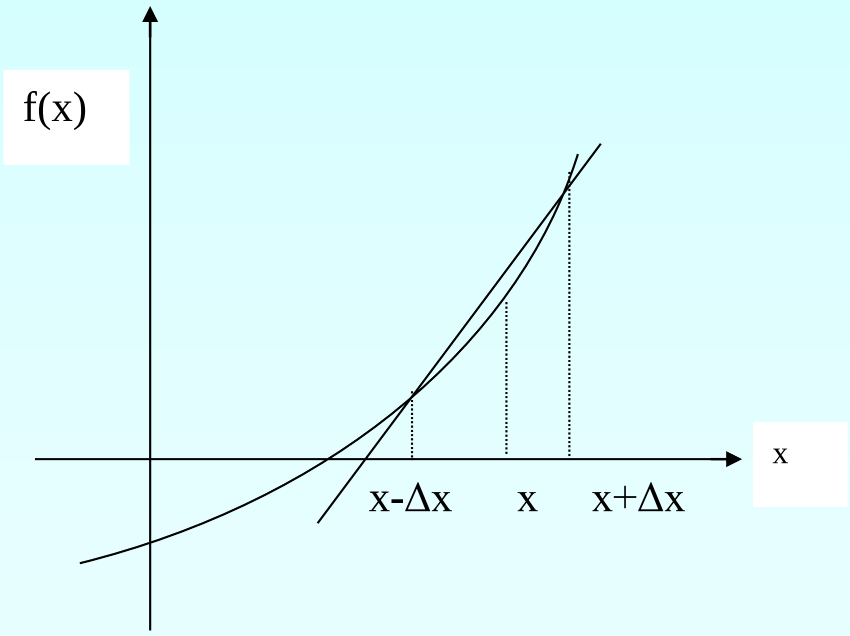


Figure 3 Graphical Representation of central difference approximation of first derivative

Example 4

The velocity of a rocket is given by

$$v(t) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t, 0 \le t \le 30$$

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 4 cont.

Solution

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

$$t_i = 16$$

$$\Delta t = 2$$

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

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

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

Example 4 cont.

$$\nu(18) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100(18)}\right] - 9.8(18)$$

$$= 453.02\,\text{m/s}$$

$$\nu(14) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100(14)}\right] - 9.8(14)$$

$$= 334.24\,\text{m/s}$$

$$a(16) \approx \frac{\nu(18) - \nu(14)}{4}$$

$$\approx \frac{453.02 - 334.24}{4}$$

$$\approx 29.694\,\text{m/s}^2$$

Example 4 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

$$|\in_t| = \left|\frac{29.674 - 29.694}{29.674}\right| \times 100$$

$$= 0.069157\,\%$$

Comparision 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)	$\lvert\in_t\rvert\%$
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

$$v(t) = 2000 \ln\left[\frac{14\times10^4}{14\times10^4 - 2100t}\right] - 9.8t$$

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	$v'(t)$	$\lvert \in_a \rvert \%$
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.

Numerical Differentiation with MATLAB

- MATLAB has built-in functions to help take derivatives, polyder, **diff and gradient**:
- polyder: returns the deriviative of a polynomial
- **diff(*x*):**Returns the difference between adjacent elements in x

Numerical Differentiation with MATLAB

- ***fx* = gradient(*f*, *h*): d**etermines the derivative of the data in f at each of the points.
- The program uses forward difference for the first point, backward difference for the last point, and centered difference for the interior points. h is the spacing between points; if omitted h=1.
- The major advantage of gradient over diff is gradient's result is the same size as the original data.
- Gradient can also be used to find partial derivatives for matrices:
  [*fx*, *fy*] = gradient(*f*, *h*)

Polynomial/Symbolic Conversions

- **sym2poly(s)** converts from a symbolic expression s to a row vector representing polynomial coefficients
- **poly2sym(p)** converts from the row vector representing polynomial coefficients p to a symbolic expression

Symbolic Expressions

- Create symbolic variables using the **sym** function, e.g.
  - a = sym(‘a’);
  - Shortcut for a lot of these: syms x y z
  - symvar = sym(‘x^3 – 2’);
- Symbolic math: doing math on symbols!
  - Using normal operators e.g. +, -, *, etc.
- Symbolic expressions are rational, e.g. kept in fractional form so sym(2/4) returns 1/2 rather than 0.5

Symbolic Functions

- **simplify** simplifies expressions
- **collect** collects like terms
- **expand** multiplies out terms
- **factor** factors a symbolic expression
- **subs** substitutes a value into an expression
- **numden** returns separately the numerator and denominator of a fraction
- **pretty** is a display function; shows exponents
- **ezplot** will draw a 2-D plot in the x-range from -2 π to 2 π

Examples

```
>> y = sym('y');
>> a = y * sym('y^2')
a =
 y^3

>> a/y
ans =
y^2

>> subs(a,4)
ans =
    64
```

```
>> 1/4 + 3/6
ans =
    0.7500

>> [n d] = numden(sym(1/4 + 3/6))
 n =
3

d =
4

>> syms a
>> expand((a+3)*(a-2))
ans =
a^2+a-6
```

Calculus: Integration/Differentiation

- **trapz**: implements the trapezoidal rule to approximate an integral
- **quad**: implements Simpson's method
- **polyint**: returns the integral of a polynomial
- **polyder**: returns the deriviative of a polynomial
- Calculus in Symbolic Math Toolbox:
  - **diff** to differentiate
  - **int** to integrate