CPNA Lecture 20 - Differentiation and Integration

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Numerical Differentiation I

- To compute the value of the derivative of a function $f(x)$, which is not defined explicitly, but its value at some finite number of points x_0, x_1, x_2, ..., x_n is given
    1. Determine an interpolating polynomial approximating the function (either on the whole interval or in sub-intervals)
    2. Differentiate this polynomial to approximately compute the value of the derivative at the given point

Numerical Differentiation II

- Consider Newton's Forward Difference Formula

$$f(x) = f(x_0) + \Delta f_0 u + \frac{\Delta^2 f_0}{2!} u(u-1) + \frac{\Delta^3 f_0}{3!} u(u-1)(u-2) + \dots$$
$$+ \frac{\Delta^n f_0}{n!} u(u-1)(u-2)\dots(u-\overline{n-1}) \text{ where, } x = x_0 + uh$$

- Then, $\frac{df}{dx} = \frac{df}{du} . \frac{du}{dx}$

$$= \frac{1}{h}\Bigg[\Delta f_0 + \frac{2u-1}{2!}\Delta^2 f_0 + \frac{3u^2-6u+2}{3!}\Delta^3 f_0 + \dots$$
$$+ \frac{\left(nu^{n-1} - \frac{n(n-1)^2}{2}u^{n-2} + \dots + (-1)^{n-1}(n-1)!\right)}{n!}\Delta^n f_0\Bigg]$$

- Thus, an approximation to the value of first derivative at $x = x_0$ i.e. $u = 0$ is obtained as

$$\left[\frac{df}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \dots + (-1)^{(n-1)}\frac{\Delta^n f_0}{n}\right]$$

Numerical Differentiation III

- Differentiating once again, we get

$$\frac{d^2 f}{dx^2} = \frac{1}{h^2}\left[\Delta^2 f_0 + \frac{6u-6}{6}\Delta^3 f_0 + \frac{12u^2-36u+22}{24}\Delta^4 f_0 + \ldots\right]$$

- An approximation to the value of second derivative at $x = x_0$ i.e. $u = 0$ is obtained as

$$\left[\frac{d^2 f}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12}\Delta^4 f_0 + \ldots\right]$$

- Formula for higher order derivatives can be obtained by successive differentiation

Numerical Differentiation IV

- Consider, Newton's backward difference formula

$$f_n(x) = f(x_n) + u\nabla f_n + \frac{u(u+1)}{2!}\nabla^2 f_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_n + \dots$$

$$\frac{df}{dx} = \nabla f_n + \frac{2u+1}{2!}\nabla^2 f_n + \frac{3u^2+6u+2}{3!}\nabla^3 f_n + \dots$$

$$\left[\frac{df}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\nabla f_n + \frac{1}{2}\nabla^2 f_n + \frac{1}{3}\nabla^3 f_n + \dots\right]$$

$$\left[\frac{d^2 f}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\nabla^2 f_n + \nabla^3 f_n + \frac{11}{12}\nabla^4 f_n + \frac{5}{6}\nabla^5 f_n \dots\right]$$

Numerical Differentiation V

- **Exercise**: The following data gives the velocity of a particle for 8 seconds at an interval of 2 seconds. Find the initial acceleration using the entire data.

x (time in sec)	0	2	4	6	8
$f(x)$(velocity in m/sec)	0	172	1304	4356	10288

- **Solution**: If v is the velocity, then initial acceleration is given by $\left[\frac{df}{dx}\right]_{x=0}$

Numerical Differentiation VI

x	$f(x)$	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$
0	0				
		172			
2	172		960		
		1132		960	
4	1304		1920		0
		3052		960	
6	4356		2880		
		5932			
8	10288				

Table 1: Forward Difference Table

Numerical Differentiation VII

We have,

$$\begin{aligned}\left[\frac{df}{dx}\right]_{x=x_0} &= \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \dots\right] \\ &= \frac{1}{2}\left[172 - \frac{1}{2}\times 960 + \frac{1}{3}\times 960\right] \\ &= \frac{1}{2}\left[172 - 480 + 320\right] \\ &= 6\end{aligned}$$

Numerical Integration I

- Compute the value of a definite integral $\int_a^b f(x)dx$, when the values of the integrand function, $y = f(x)$ are given at some tabular points
  1. The integrand is first replaced with an interpolating polynomial
  2. Then the integrating polynomial is integrated to compute the value of the definite integral

General Approaches for Numerical Integration I

- Replace a complicated function or tabulated data with an approximating function that is easy to integrate:

$$I = \int_{x_0}^{x_n} f(x)dx \cong \int_{x_0}^{x_n} f_n(x)dx$$

where, $f_n(x)$ is a polynomial of the form

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

and n is the order of the polynomial

General Approaches for Numerical Integration II

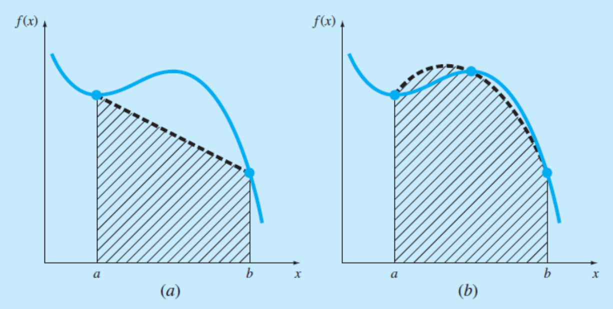

Figure 1: The approximation of an integral by the area under (a) a single straight line and (b) a single parabola

- The integral can also be approximated using a series of polynomials applied piecewise to the function or data over segments of constant length

General Approaches for Numerical Integration III

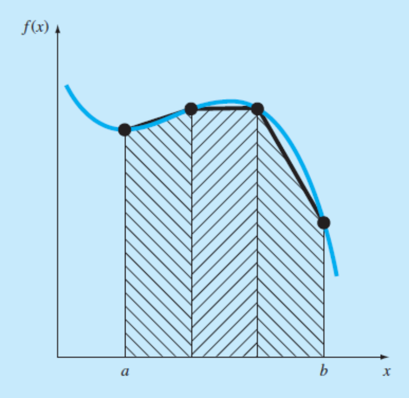

Figure 2: The approximation of an integral by the area under three straight-line segments.

- Higher-order polynomials can be utilized for the same purpose

General Approaches for Numerical Integration IV

- Closed and open forms
  - The closed forms are those where the data points at the beginning and end of the limits of integration are known
  - The open forms have integration limits that extend beyond the range of the data (similar to extrapolation)

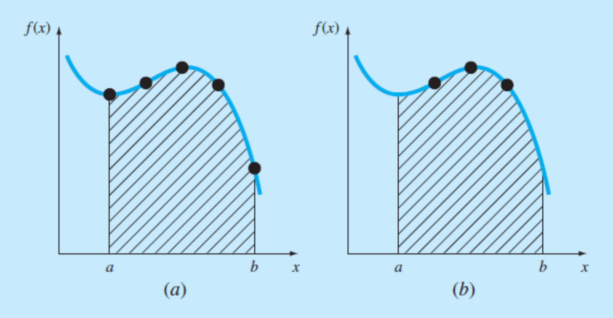

Figure 3: The difference between (a) closed and (b) open integration formulas

Methods Based on Difference Polynomials I

- We assume that the value of the integrand is given at equidistant points $a = x_0 < x_1 < x_2 < \ldots < x_n = b$
- Clearly, $x_n = x_0 + nh$, hence the integral becomes:

$$I = \int_{x_0}^{x_n} f(x)dx$$

- Any of the forward, or backward difference interpolating polynomials may be integrated to give an approximation to integral
- We use Newton's Forward Difference Formula to approximate $f(x)$,

$$I = \int_{x_0}^{x_n} \left[f(x_0) + \Delta f_0 u + \frac{\Delta^2 f_0}{2!} u(u-1) + \frac{\Delta^3 f_0}{3!} u(u-1)(u-2) + \ldots \right] dx$$

Methods Based on Difference Polynomials II

- Since, $x = x_0 + uh$, $dx = h\ du$, hence the above integral becomes

$$I = \int_{x_0}^{x_n} f(x)dx$$

$$= h \int_0^n \left[f(x_0) + \Delta f_0 u + \frac{\Delta^2 f_0}{2!} u(u-1) + \frac{\Delta^3 f_0}{3!} u(u-1)(u-2) + \dots \right] du$$

- On simplification, it becomes

$$\int_{x_0}^{x_n} f(x)dx = nh \left[f(x_0) + \frac{n}{2}\Delta f_0 + \frac{n(2n-3)}{12}\Delta^2 f_0 + \frac{n(n-2)^2}{24}\Delta^3 f_0 + \dots \right]$$

- Different integration formulae are obtained by putting $n = 1, 2, 3, \dots$ into the above general formula

Trapezoidal Method I

- Setting $n = 1$ in the general formula, we get

$$\int_{x_0}^{x_1} f(x)dx = h\left[f(x_0) + \frac{1}{2}\Delta f_0\right] = h\left[f(x_0) + \frac{1}{2}\left(f(x_1) - f(x_0)\right)\right] = \frac{h}{2}\left[f(x_0) + f(x_1)\right]$$

- Similarly, for the subsequent intervals, we get

$$\int_{x_1}^{x_2} f(x)dx = \frac{h}{2}\left[f(x_1) + f(x_2)\right], \ldots, \int_{x_{n-1}}^{x_n} f(x)dx = \frac{h}{2}\left[f(x_{n-1}) + f(x_n)\right]$$

- Combining all these, we get

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{2}\left[f(x_0) + 2(f(x_1) + f(x_2) + \ldots) + f(x_n)\right]$$

Trapezoidal Method II

- Geometrical interpretation
  - Curve $y = f(x)$ is replaced by n straight lines joining the points (x_0, y_0) and (x_1, y_1); (x_1, y_1) and (x_2, y_2); . . . ; (x_{n-1}, y_{n-1}) and (x_n, y_n)
  - The area bounded by the curve $y = f(x)$, the ordinates $x = x_0$, $x = x_n$ and the x-axis is then approximately equal to the sum of the areas of the n trapeziums obtained

Trapezoidal Method III

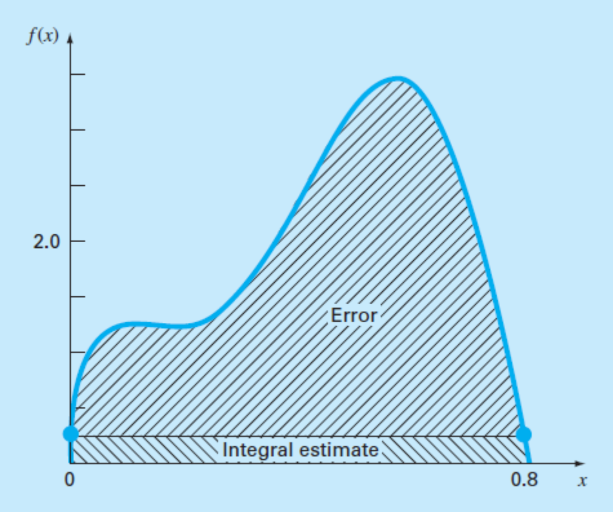

Figure 4: Single application of the trapezoidal rule to approximate the integral of $f(x)$

Trapezoidal Method IV

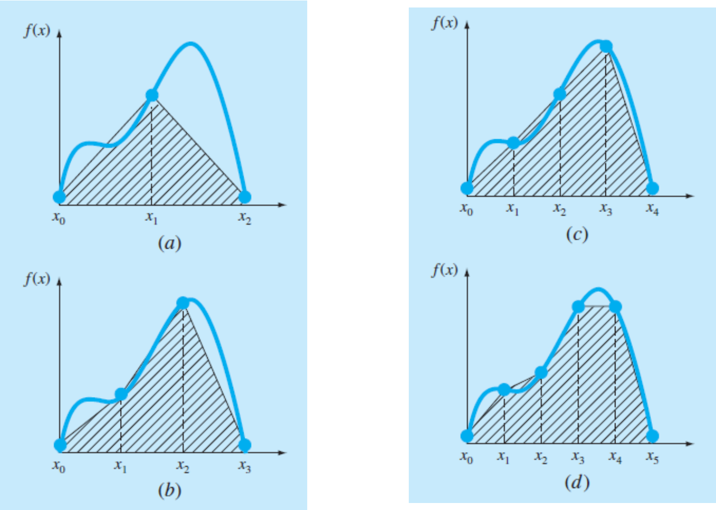

Figure 5: Multiple Applications of Trapezoidal Rule

Trapezoidal Method V

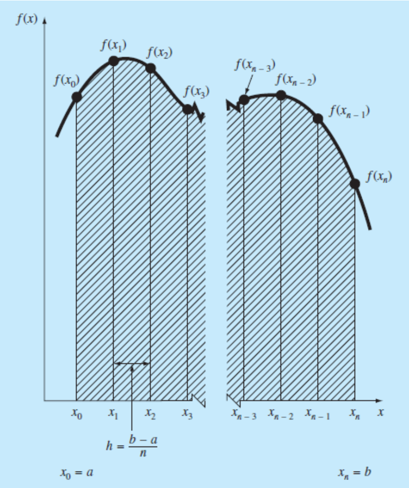

Figure 6: Multiple Applications of Trapezoidal Rule - General Form

Simpson's Meothod I

- To obtain a more accurate estimate of an integral, use higher-order polynomials to connect the points
- Simpson's $1/3^{rd}$ rule results when a second-order interpolating polynomial is used

$$I = \int_{x_0}^{x_n} f(x)dx \cong \int_{x_0}^{x_n} f_2(x)dx$$

- Setting $n = 2$ in the general formula, we get

$$\int_{x_0}^{x_2} f(x)dx = 2h\left[f(x_0) + \Delta f_0 + \frac{1}{6}\Delta^2 f_0\right] = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$

Simpson's Meothod II

- Similarly,

$$\int_{x_2}^{x_4} f(x)dx = \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right]$$

$$\cdots$$

$$\int_{x_{n-2}}^{x_n} f(x)dx = \frac{h}{3}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]$$

- Summing up we get

$$\int_{x_0}^{x_n} f(x)dx = \frac{h}{3}\left[f(x_0) + 4\left(f(x_1) + f(x_3) + \ldots + f(x_{n-1})\right)\right.$$
$$\left. + \; 2\left(f(x_2) + f(x_4) + \ldots + f(x_{n-2})\right) + f(x_n)\right]$$

Simpson's Meothod III

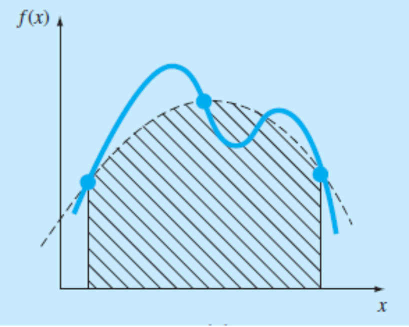

Figure 7: Single Application of Simpson's 1/3 rule:

Simpson's Meothod IV

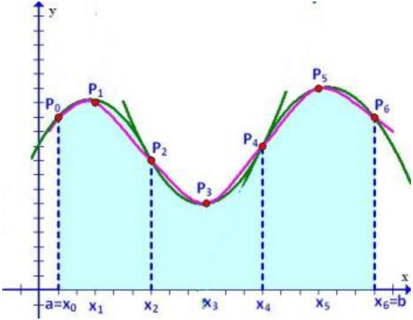

Figure 8: Multiple Applications of Simpson's $1/3$ rule:

Example I

- **Exercise**: Approximate the integral of $f(x) = x^3$ on the interval $[1, 2]$ with four subintervals using Trapizoidal method.
- **Solution**: First, $h = (2-1)/4 = 0.25$, and thus we calculate:

$$\begin{aligned}\int_1^2 f(x)\ dx &= \frac{0.25}{2}\left[f(1) + 2(f(1.25) + f(1.5) + f(1.75)) + f(2)\right] \\ &= 3.7968\end{aligned}$$

If we double the number of intervals, that is, eight, we set $h = (2-1)/8 = 0.125$, and thus we calculate:

$$\begin{aligned}\int_1^2 f(x)\ dx &= \frac{0.125}{2}[f(1) + 2(f(1.125) + f(1.25) + f(1.375) \\ &\quad + f(1.5) + f(1.625) + f(1.75) + f(1.875)) + f(2)] \\ &= 3.76171875\end{aligned}$$

Example II

The second approximation is much closer to the correct answer of 3.75.

- **Exercise**: The velocity of a particle which starts from rest is given by the following table

t	0	2	4	6	8	10	12	14	16	18	20
$v(ft/sec)$	0	16	29	40	46	51	32	18	8	3	0

Evaluate using Trapezium rule and Simpson's 1/3 rule, the total distance travelled in 20 seconds.

- **Solution**: From the definition, we have

$$v = \frac{ds}{dt}$$

or

$$s = \int v \; dt$$

Example III

Starting from rest, the distance travelled in 20 seconds is

$$s = \int_0^{20} v \ dt$$

The step length $h = 2$. Using the Trapezium rule, we obtain

$$\begin{aligned} s &= \frac{h}{2}\left[f(0) + 2(f(2) + f(4) + f(6) + f(8) + f(10) + f(12)\right. \\ &\qquad \left. f(14) + f(16) + f(18)) + f(20)\right] \\ &= 0 + (16 + 29 + 40 + 46 + 51 + 32 + 18 + 8 + 3) + 0 \\ &= 486 \ ft \end{aligned}$$

Using the Simpson's $1/3$ rule, we obtain

Example IV

$$
\begin{aligned}
s &= \frac{h}{3}\left[f(0) + 4(f(2) + f(6) + f(10) + f(14) + f(18))\right. \\
&\qquad \left. + 2(f(4) + f(8) + f(12) + f(16)) + f(20)\right] \\
&= \frac{2}{3}\left[0 + 4(16 + 40 + 51 + 18 + 3) + 2(29 + 46 + 32 + 8) + 0\right] \\
&= 494.667\ ft
\end{aligned}
$$