ENGINEERING MATHEMATICS II

010.141

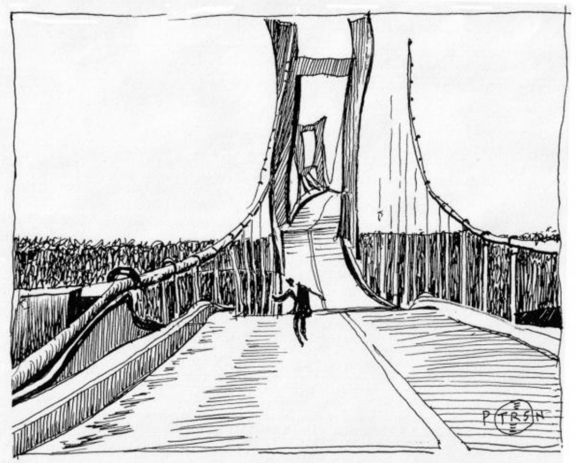
NUMERICAL METHODS IN GENERAL

MODULE 5

NUMERICAL METHODS

- Methods for solving problems numerically on a computer
- **Steps**:
  - Modeling,
  - Choice of a numerical method, Programming,
  - Doing the computation,
  - Interpreting the results
- Solution of equations by iteration
- Interpolation
- Numerical integration and differentiation

Nonlinear Equations in Engineering Fields



$f(x) = \omega_n(x) - \omega = 0$
x: bridge design variables

To design a safe bridge , a natural frequency must be higher than that of an external loading.

$f(x) = T(x) - T^* = 0$
x: battery design variables

To design a safe battery, a temperature level must be smaller than a marginal temperature.

$f(x) = \sigma(x) - S = 0$
x: bridge gusset plate

To design a safe bridge, a stress level at a critical bridge element must be smaller than its strength.

SOLUTION OF EQUATIONS BY ITERATION

- Solving equation f(x) = 0
- **Methods**:
  - Fixed – Point Iteration
  - Newton's Method
  - Secant Method

FIXED-POINT ITERATION FOR SOLVING $f(x) = 0$

- **Idea**: transform $f(x) = 0$ into $x = g(x)$
- **Steps**:
  1. Choose x_0
  2. Compute $x_1 = g(x_0)$, $x_2 = g(x_1)$, …, $x_{n+1} = g(x_n)$
- A solution of $x = g(x)$ is called a **fixed point**
- Depending on the initial value chosen (x_0), the related sequences may converge or diverge

FIXED-POINT ITERATION FOR SOLVING f(x) = 0

- **Example**: $f(x) = x^2 - 3x + 1 = 0$

$$\text{Solutions} = \begin{cases} 2.618034 \\ 0.381966 \end{cases}$$

The equation may be written

(4a) $$x = g_1(x) = \frac{1}{3}(x^2 + 1), \qquad \text{thus} \qquad x_{n+1} = \frac{1}{3}(x_n^2 + 1).$$

If we choose $x_0 = 1$, we obtain the sequence (Fig. 423a; computed with 6S and then rounded)

$$x_0 = 1.000, \quad x_1 = 0.667, \quad x_2 = 0.481, \quad x_3 = 0.411, \quad x_4 = 0.390, \cdots$$

which seems to approach the smaller solution. If we choose $x_0 = 2$, the situation is similar. If we choose $x_0 = 3$, we obtain the sequence (Fig. 423a, upper part)

$$x_0 = 3.000, \quad x_1 = 3.333, \quad x_2 = 4.037, \quad x_3 = 5.766, \quad x_4 = 11.415, \cdots$$

which diverges.

FIXED-POINT ITERATION FOR SOLVING f(x) = 0

Our equation may also be written (divide by x)

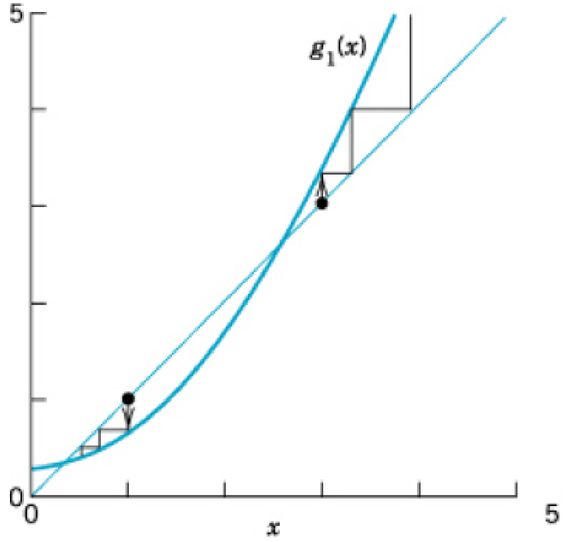
(4b) $$x = g_2(x) = 3 - \frac{1}{x}, \qquad \text{thus} \qquad x_{n+1} = 3 - \frac{1}{x_n},$$

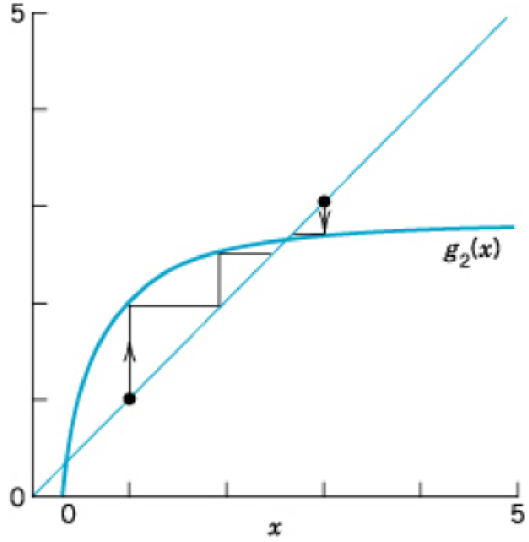
and if we choose $x_0 = 1$, we obtain the sequence (Fig. 423b)

$$x_0 = 1.000, \quad x_1 = 2.000, \quad x_2 = 2.500, \quad x_3 = 2.600, \quad x_4 = 2.615, \cdots$$

which seems to approach the larger solution. Similarly, if we choose $x_0 = 3$, we obtain the sequence (Fig. 423b)

$$x_0 = 3.000, \quad x_1 = 2.667, \quad x_2 = 2.625, \quad x_3 = 2.619, \quad x_4 = 2.618, \cdots$$





NEWTON'S METHOD FOR SOLVING f(x) = 0

- f must have a continuous derivative f '
- The method is simple and fast

$$\tan\beta = f'(x_0) = \frac{f(x_0)}{x_0 - x_1}$$

$$\Downarrow$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

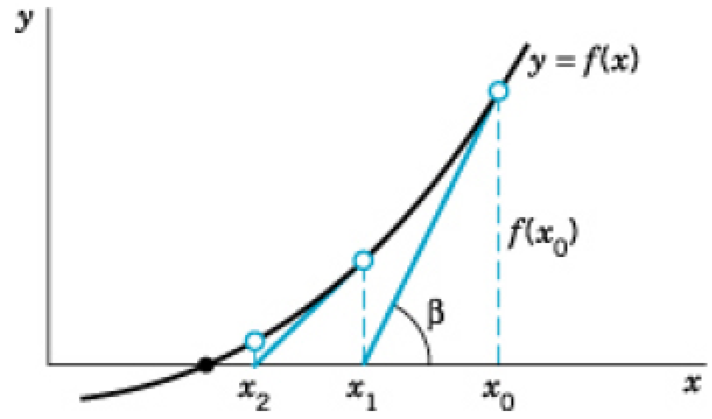


Fig. 425. Newton's method

NEWTON'S METHOD FOR SOLVING f(x) = 0

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)}$$

$$\vdots$$

$$\boxed{x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}}$$

NEWTON'S METHOD FOR SOLVING f(x) = 0

Example: Find the positive solution of f(x) = 2 sin x – x = 0

Solution:

Setting $f(x) = x - 2\sin x$, we have $f'(x) = 1 - 2\cos x$, and (5) gives

$$x_{n+1} = x_n - \frac{x_n - 2\sin x_n}{1 - 2\cos x_n} = \frac{2(\sin x_n - x_n \cos x_n)}{1 - 2\cos x_n} = \frac{N_n}{D_n}.$$

From the graph of f we conclude that the solution is near $x_0 = 2$. We compute:

n	x_n	N_n	D_n	x_{n+1}
0	2.00000	3.48318	1.83229	1.90100
1	1.90100	3.12470	1.64847	1.89552
2	1.89552	3.10500	1.63809	1.89550
3	1.89550	3.10493	1.63806	1.89549

$x_4 = 1.89549$ is exact to 5D since the solution to 6D is 1.895 494.

SECANT METHOD FOR SOLVING f(x) = 0

Newton's method is powerful but disadvantageous because it is difficult to obtain f '. The secant method approximates f '.

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

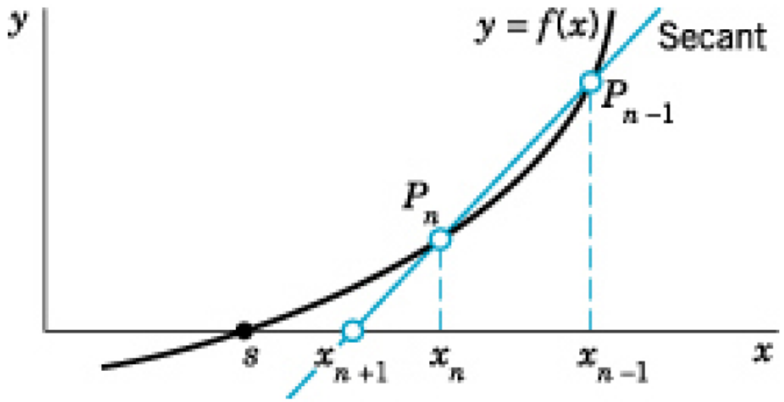


Fig. 426. Secant method

SECANT METHOD FOR SOLVING f(x) = 0

- Newton's Method

$$x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$$

- Secant

$$f'(x_n) \approx \frac{f(x_n) - f(x_{n-1})}{x_n - x_{n-1}}$$

$$\Downarrow$$

$$x_{n+1} = x_n - f(x_n)\frac{x_n - x_{n-1}}{f(x_n) - f(x_{n-1})}$$

SECANT METHOD FOR SOLVING f(x) = 0

Find the positive solution of $f(x) = x - 2\sin x = 0$ by the secant method, starting from $x_0 = 2$, $x_1 = 1.9$.

Solution:

Here, (10) is

$$x_{n+1} = x_n - \frac{(x_n - 2\sin x_n)(x_n - x_{n-1})}{x_n - x_{n-1} + 2(\sin x_{n-1} - \sin x_n)} = x_n - \frac{N_n}{D_n}.$$

Numerical values are:

n	x_{n-1}	x_n	N_n	D_n	$x_{n+1} - x_n$
1	2.000 000	1.900 000	−0.000 740	−0.174 005	−0.004 253
2	1.900 000	1.895 747	−0.000 002	−0.006 986	−0.000 252
3	1.895 747	1.895 494	0		0

$x_3 = 1.895\ 494$ is exact to 6D. See Example 4.

진정성이 마음을 움직인다.

송나라 범관, 계산행려도

INTERPOLATION

- Function f(x) is unknown
- Some values of f(x) are known (f_1, f_2, …, f_n)
- **Idea**: Find a polynomial $p_n(x)$ that is an approximation of f(x)

$$\boxed{p_n(x_0) = f_0,\ p_n(x_1) = f_1,\ \cdots,\ p_n(x_n) = f_n}$$

- **Lagrange interpolation**
  - Linear
  - Quadratic
  - General
- **Newton's interpolation**
  - Divided difference
  - Forward difference
  - Backward difference
- **Splines**

LINEAR LAGRANGE INTERPOLATION

- Use 2 known values of f(x) $\rightarrow$ f_0, f_1

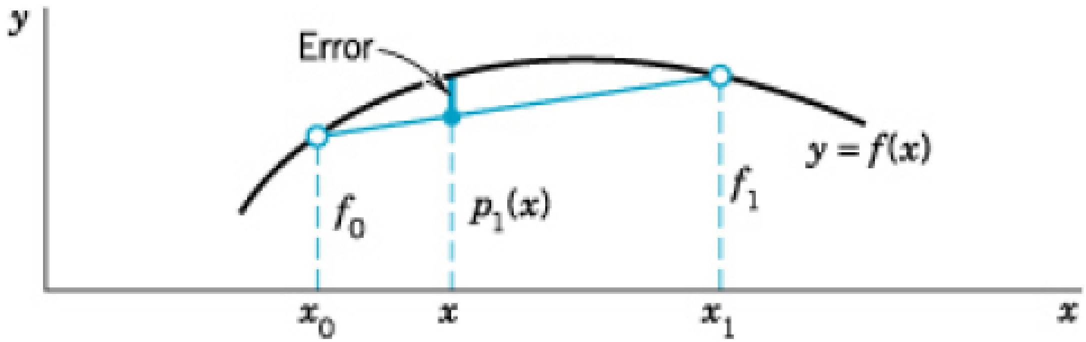


Fig. 428. Linear interpolation

p_1 is the linear Lagrange polynomial.

LINEAR LAGRANGE INTERPOLATION

- $p_1(x) = L_0(x)f_0 + L_1(x)f_1$
- L_0 and L_1 are linear polynomials (weight functions).

$$L_0(x) = \begin{cases} 1 \text{ if } x = x_0 \\ 0 \text{ if } x = x_1 \end{cases} \qquad L_1(x) = \begin{cases} 0 \text{ if } x = x_0 \\ 1 \text{ if } x = x_1 \end{cases}$$

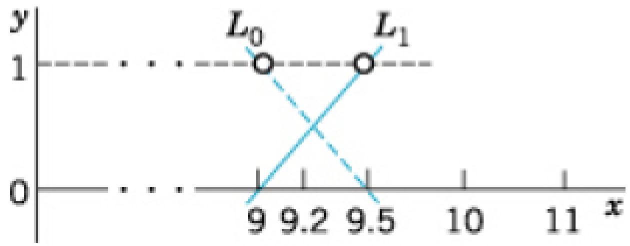


Fig. 429. L_0 and L_1 in Example 1

$$L_0(x) = \frac{x - x_1}{x_0 - x_1}, \quad L_1(x) = \frac{x - x_0}{x_1 - x_0}$$

$$\boxed{p_1(x) = \frac{x - x_1}{x_0 - x_1} f_0 + \frac{x - x_0}{x_1 - x_0} f_1}$$

LINEAR LAGRANGE INTERPOLATION

Example: Compute ln 9.2 from ln 9.0 = 2.1972 and ln 9.5 = 2.2513 by linear Lagrange interpolation

Solution:

$$x_0 = 9.0, \quad x_1 = 9.5, \quad f_0 = \ln 9.0, \quad f_1 = \ln 9.5$$

$$L_0(9.2) = \frac{9.2 - 9.5}{9.0 - 9.5} = 0.6 \qquad L_1(9.2) = \frac{9.2 - 9.0}{9.5 - 9.0} = 0.4$$

$$\begin{aligned}\ln 9.2 &\approx p_1(9.2) \\ &= L_0(9.2) f_0 + L_1(9.2) f_1 \\ &= 0.6(2.1972) + 0.4(2.2513) \\ &= 2.2188\end{aligned}$$

$$\text{Error}: \quad \ln 9.2 - p_1(9.2) = 2.2192 - 2.2188 = 0.0004$$

QUADRATIC LAGRANGE INTERPOLATION

- Use of 3 known values of f(x) → f_0, f_1, f_2
- Approximation of f(x) by a second-degree polynomial

$$p_2(x) = L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2$$

$$L_0 = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)}$$

$$L_1 = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)}$$

$$L_2 = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

QUADRATIC LAGRANGE INTERPOLATION

Example: Compute ln 9.2 for f_0 (x_0 = 9.0) = ln 9.0, f_1 (x_1 = 9.5) = ln 9.5, f_2 (x_2 = 11.0) = ln 11.0

Solution:

$$L_0(x) = x^2 - 20.5x + 104.5$$

$$L_1(x) = -\frac{1}{0.75}\left(x^2 - 20x + 99\right)$$

$$L_2(x) = \frac{1}{3}\left(x^2 - 18.5x + 85.5\right)$$

$$\ln 9.2 \approx p_2(9.2) = 2.2192$$

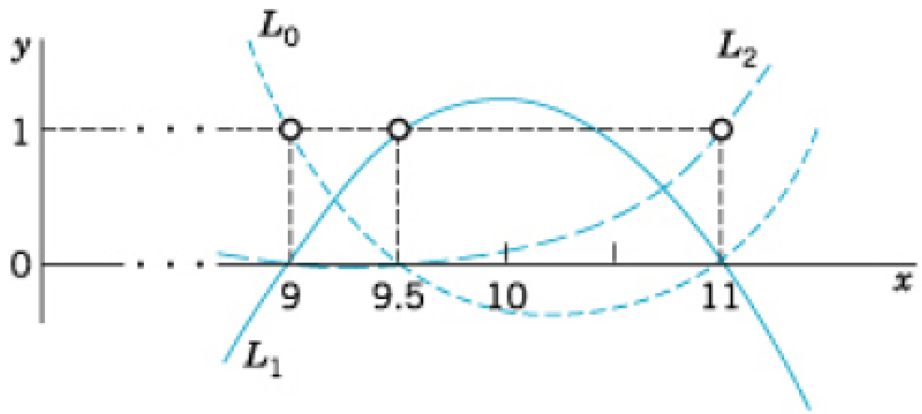


Fig. 430. L_0, L_1, L_2 in Example 2

GENERAL LAGRANGE INTERPOLATION

$$f(x) \approx p_n(x) = \sum_{\mathrm{k}=0}^{n} \mathrm{L}_{\mathrm{k}}(x) f_k$$

$$= \sum_{\mathrm{k}=0}^{n} \frac{l_{\mathrm{k}}(x)}{l_{\mathrm{k}}(x_k)} f_k$$

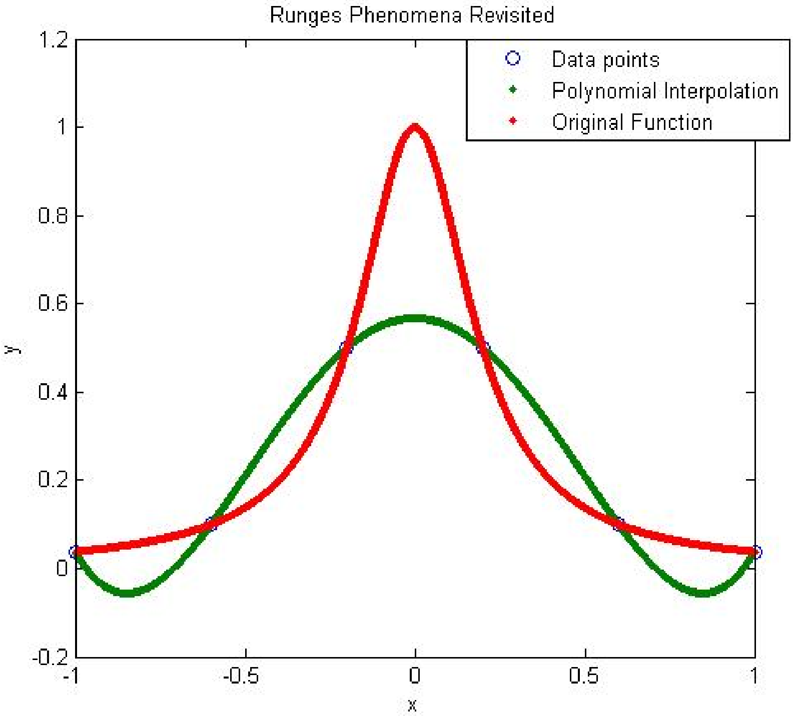
$$l_{\mathrm{k}}(x) = (x - x_0)\cdots(x - x_{k-1})(x - x_{k+1})\cdots(x - x_n)$$

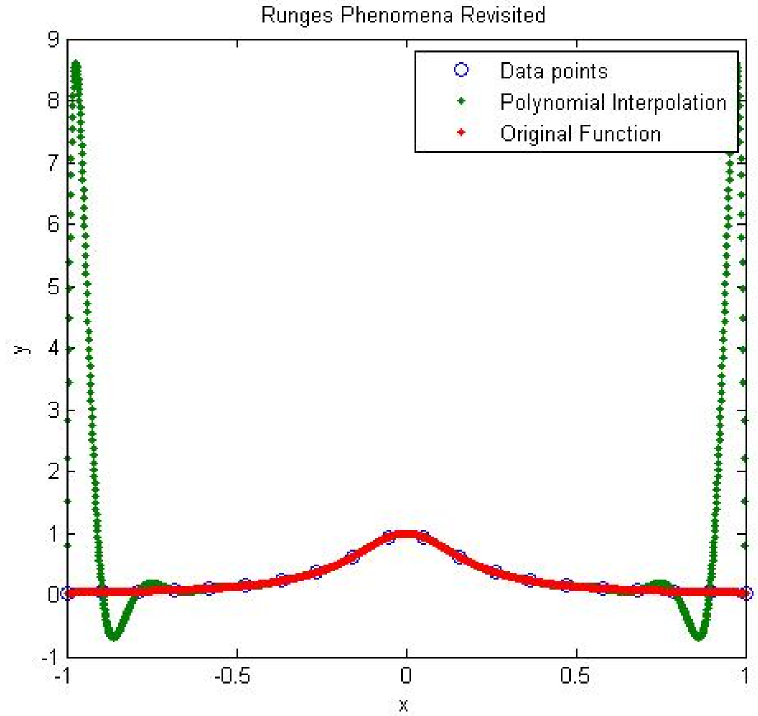
NEWTON'S INTERPOLATION

- More appropiate for computation
- Level of accuracy can be easily improved by adding new terms that increase the degree of the polynomial
- Divided difference
- Forward difference
- Backward difference

Is High-Order Polynomial a Good Idea?

$$f(x) = 1/(1+25x^2)$$





SPLINES

- Method of interpolation used to avoid numerical instability

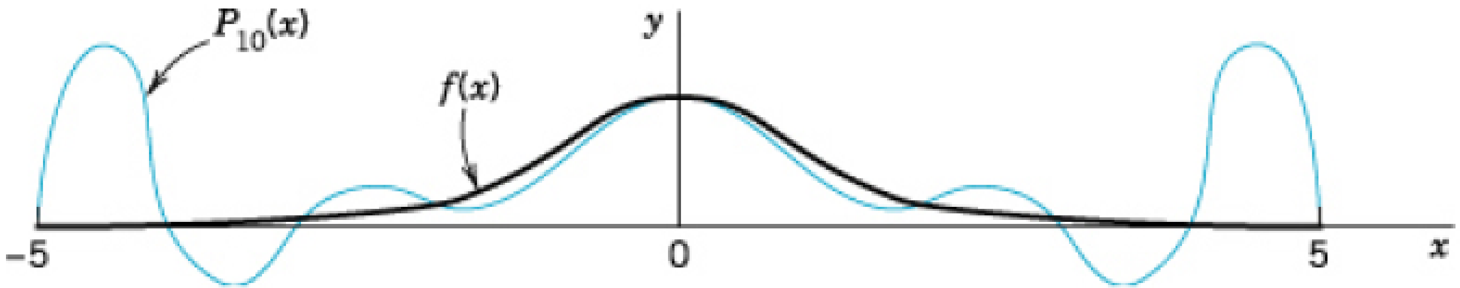


Fig. 431. Runge's example $f(x) = 1/(1 + x^2)$ and interpolating polynomial $P_{10}(x)$

- **Idea**: given an interval [a, b] where the high-degree polynomial can oscillate considerable, we subdivide [a, b] in several smaller intervals and use several low-degree polynomials (which cannot oscillate much)

SPLINES (cont)

- In an interval $x \in [x_j, x_{j+1}]$, $j = 0, \ldots, n-1$

$$\boxed{p_j(x) = a_{j_0} + a_{j_1}(x - x_j) + a_{j_2}(x - x_j)^2 + a_{j_3}(x - x_j)^3}$$

where

$$a_{j0} = p_j(x_j) = f_j$$

$$a_{j1} = p'_j(x_j) = k_j$$

$$a_{j2} = \frac{1}{2}p''_j(x_j) = \frac{3}{h^2}\left(f_{j+1} - f_j\right) - \frac{1}{h}\left(k_{j+1} + 2k_j\right)$$

$$a_{j3} = \frac{2}{h^3}\left(f_j - f_{j+1}\right) + \frac{1}{h^2}\left(k_{j+1} + k_j\right)$$

SPLINES (cont)

- Let (x_0,f_0), (x_1,f_1), … , (x_n,f_n).
- k_0, k_n are two given numbers.
- $k_1, k_2, \ldots, k_{n-1}$ are determined by a linear system of n-1 equations:

$$k_{j-1} + 4k_j + k_{j+1} = \frac{3}{h}\left(f_{j+1} - f_{j-1}\right)$$

$$p'_j\left(x_j\right) = k_j, \quad p'_j\left(x_j + 1\right) = k_{j+1} \quad \left(\mathrm{j} = 0, 1, \ldots, \mathrm{n-1}\right)$$

- h is the distance between nodes

$$x_n = x_0 + nh$$

SPLINES (cont)

- Clamped conditions

$$g'(x_0) = f'(x_0), \quad g'(x_n) = f'(x_n)$$

- Free/natural conditions

$$g''(x_0) = 0, \quad g''(x_n) = 0$$

- **Example**:

  Interpolate $f(x) = x^4$ on interval $x \in [-1, 1]$ by cubic spline in partitions $x_0 = -1$, $x_1 = 0$, $x_2 = 1$, satisfying clamped conditions

$$g'(-1) = f'(-1), \quad g'(1) = f'(1)$$

SPLINES (cont)

the given data are $f_0 = f(-1) = 1, f_1 = f(0) = 0, f_2 = f(1) = 1.$

$$q_0(x) = a_{00} + a_{01}(x+1) + a_{02}(x+1)^2 + a_{03}(x+1)^3 \quad (-1 \leqq x \leqq 0)$$
$$q_1(x) = a_{10} + a_{11}x + a_{12}x^2 + a_{13}x^3 \quad (0 \leqq x \leqq 1)$$

$$k_0 + 4k_1 + k_2 = 3(f_2 - f_0) .$$

Here $f_0 = f_2 = 1$ (the value of x^4 at the ends) and $k_0 = -4,\ k_2 = 4,$

$$-4 + 4k_1 + 4 = 3(1-1) = 0, \qquad k_1 = 0$$

$$a_{00} = f_0 = 1,\ a_{01} = k_0 = -4$$

$$a_{02} = \frac{3}{1^2}(f_1 - f_0) - \frac{1}{1}(k_1 + 2k_0) = 3(0-1) - (0-8) = \quad 5$$

$$a_{03} = \frac{2}{1^3}(f_0 - f_1) + \frac{1}{1^2}(k_1 + k_0) = 2(1-0) + (0-4) = -2 .$$

SPLINES (cont)

Similarly, for the coefficients of q_1 we obtain from (13) the values $a_{10} = f_1 = 0$, $a_{11} = k_1 = 0$, and

$$a_{12} = 3(f_2 - f_1) - (k_2 + 2k_1) = 3(1-0) - (4+0) = -1$$

$$a_{13} = 2(f_1 - f_2) + (k_2 + k_1) = 2(0-1) + (4+0) = 2\,.$$

This gives the polynomials of which the spline $g(x)$ consists, namely,

$$g(x) = \begin{cases} q_0(x) = 1 - 4(x+1) + 5(x+1)^2 - 2(x+1)^3 = -x^2 - 2x^3 & \text{if} \quad -1 \leqq x \leqq 0 \\ q_1(x) = -x^2 + 2x^3 & \text{if} \quad 0 \leqq x \leqq 1\,. \end{cases}$$

Figure 433 shows $f(x)$ and this spline. Do you see that we could have saved over half of our work by using symmetry?

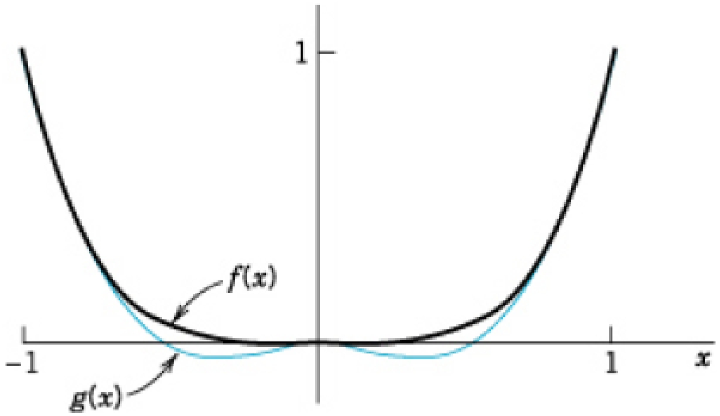


Fig. 433. Function $f(x) = x^4$ and cubic spline $g(x)$ in Example 1

NUMERICAL INTEGRATION

- Numerical evaluation of integrals whose analytical evaluation is too complicated or impossible, or that are given by recorded numerical values

$$\int_a^b f(x)dx$$

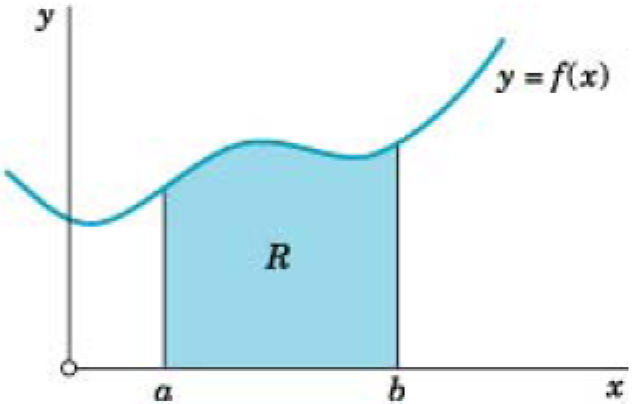


Fig. 437. Geometric interpretation of a definite integral

- Rectangular rule
- Trapezoidal rule
- Simpson's rule
- Gauss integration

RECTANGULAR RULE

- Approximation by n rectangular areas

$$J = \int_a^b f(x)dx \approx h\left[f(x^*_1) + f(x^*_2) + \cdots + f(x^*_n)\right]$$

where

$$h = \frac{b-a}{n}$$

$$x_1 = x_0 + h$$

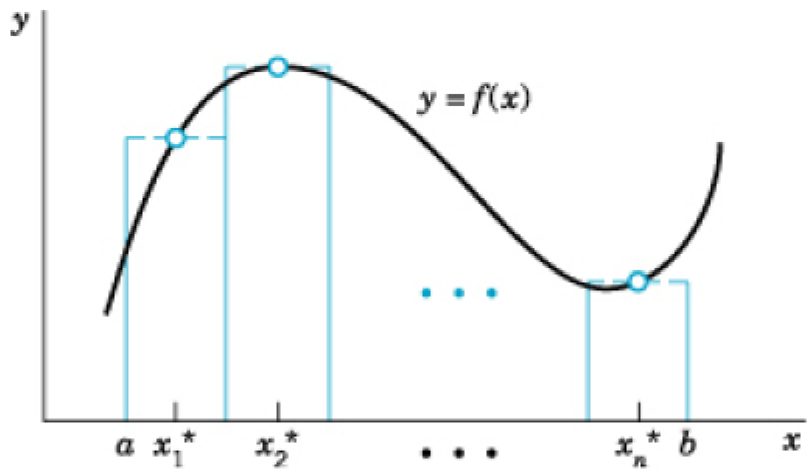


Fig. 438. Rectangular rule

TRAPEZOIDAL RULE

- Approximation by n trapezoidal areas

$$J = \int_a^b f(x)dx \approx h\left[\frac{1}{2}f(a) + f(x_1) + f(x_2) + \cdots + f(x_{n-1}) + \frac{1}{2}f(b)\right]$$

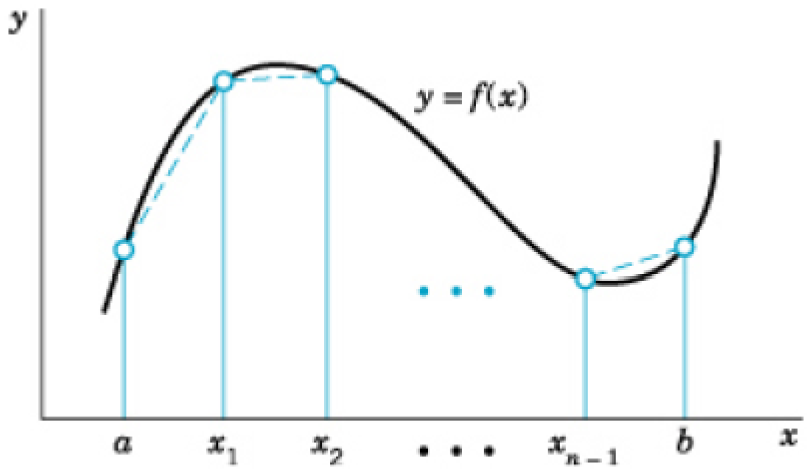


Fig. 439. Trapezoidal rule

TRAPEZOIDAL RULE

Evaluate $J = \int_0^1 e^{-x^2} dx$ by means of (2) with $n = 10$.

Solution:

$J \approx 0.1(0.5 \cdot 1.367\,879 + 6.778\,167) = 0.746\,211$ from Table 19.3.

TABLE 19.3 Computations in Example 1

j	x_j	x_j^2	$e^{-x_j^2}$	
0	0	0	1.000 000	
1	0.1	0.01		0.990 050
2	0.2	0.04		0.960 789
3	0.3	0.09		0.913 931
4	0.4	0.16		0.852 144
5	0.5	0.25		0.778 801
6	0.6	0.36		0.697 676
7	0.7	0.49		0.612 626
8	0.8	0.64		0.527 292
9	0.9	0.81		0.444 858
10	1.0	1.00	0.367 879	
Sums			1.367 879	6.778 167

SIMPSON'S RULE

- Approximation by parabolas using Lagrange polynomials $p_2(x)$
- Interval of integration [a, b] divided into an even number of subintervals

$$h = \frac{b-a}{2m} \qquad f_0 = f(x_0) \qquad x_1 = a + h \qquad x_2 = x_1 + h$$

$$\int_a^b f(x)dx \approx \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{2m-2} + 4f_{2m-1} + f_{2m}\right)$$

$$f_j = f(x_j)$$

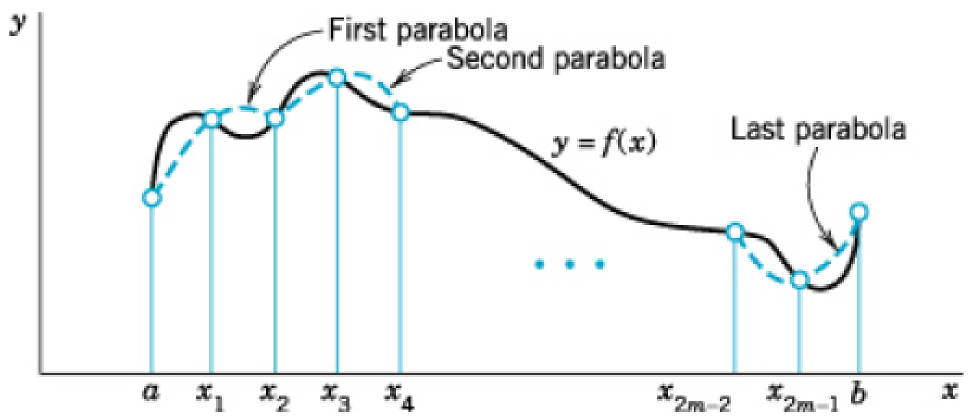


Fig. 440. Simpson's rule

SIMPSON'S RULE

Evaluate $J = \int_0^1 e^{-x^2} dx$ by Simpson's rule with $2m = 10$ and estimate the error.

Solution:

Since $h = 0.1$, Table 19.5 gives

$$J \approx \frac{0.1}{3}(1.367\ 879 + 4 \cdot 3.740\ 266 + 2 \cdot 3.037\ 901) = 0.746\ 825\,.$$

TABLE 19.5 **Computations in Example 3**

j	x_j	x_j^2	$e^{-x_j^2}$		
0	0	0	1.000 000		
1	0.1	0.01		0.990 050	
2	0.2	0.04			0.960 789
3	0.3	0.09		0.913 931	
4	0.4	0.16			0.852 144
5	0.5	0.25		0.778 801	
6	0.6	0.36			0.697 676
7	0.7	0.49		0.612 626	
8	0.8	0.64			0.527 292
9	0.9	0.81		0.444 858	
10	1.0	1.00	0.367 879		
Sums			1.367 879	3.740 266	3.037 901

SIMPSON'S RULE

ALGORITHM SIMPSON $(a, b, m, f_0, f_1, \cdots, f_{2m})$

This algorithm computes the integral $J = \int_a^b f(x)\,dx$ from given values $f_j = f(x_j)$ at equidistant $x_0 = a,\ x_1 = x_0 + h, \cdots, x_{2m} = x_0 + 2mh = b$ by Simpson's rule (7), where $h = (b - a)/(2m)$.

INPUT: $a, b, m, f_0, \cdots, f_{2m}$

OUTPUT: Approximate value $\widetilde{J}$ of J

Compute $s_0 = f_0 + f_{2m}$

$$s_1 = f_1 + f_3 + \cdots + f_{2m-1}$$

$$s_2 = f_2 + f_4 + \cdots + f_{2m-2}$$

$$h = (b - a)/2m$$

$$\widetilde{J} = \frac{h}{3}(s_0 + 4s_1 + 2s_2)$$

OUTPUT $\widetilde{J}$. Stop.

End SIMPSON

ADAPTIVE INTEGRATION

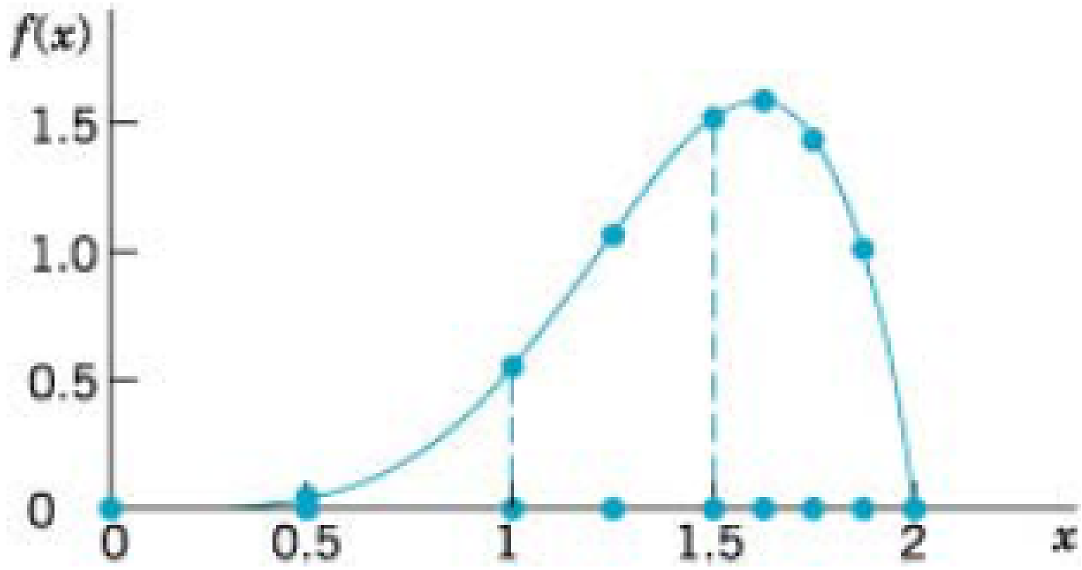


Fig. 441. Adaptive integration in Example 6

GAUSS INTEGRATION

$$\int_a^b f(x)dx = \int_{-1}^{1} f(t)dt \approx \sum_{j=1}^{\infty} A_j f_j$$

where

$$x = \frac{1}{2}\left[a(t-1) + b(t+1)\right]$$

$$A_1, \ldots, A_n \quad \Rightarrow \quad \text{coefficients}$$

$$f_j = f(t_j)$$

TABLE 19.7 **Gauss Integration: Nodes t_j and Coefficients A_j**

n	Nodes t_j	Coefficients A_j	Degree of Precision
2	−0.57735 02692	1	3
	0.57735 02692	1	
3	−0.77459 66692	0.55555 55556	5
	0	0.88888 88889	
	0.77459 66692	0.55555 55556	
4	−0.86113 63116	0.34785 48451	7
	−0.33998 10436	0.65214 51549	
	0.33998 10436	0.65214 51549	
	0.86113 63116	0.34785 48451	
5	−0.90617 98459	0.23692 68851	9
	−0.53846 93101	0.47862 86705	
	0	0.56888 88889	
	0.53846 93101	0.47862 86705	
	0.90617 98459	0.23692 68851	