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Ngày 6 tháng 11 năm 2015

Modeling and Simulation of Physical Processes

- Describe the physical phenomenon
- Model the physical phenomenon to become mathematical equations (PDE)
- Simulate the mathematical equations (discrete solution)
- Compare the discrete solution and experiment result

Example

Equations for conservation law of mass and momentum

$$\begin{cases} \partial_t \rho + \partial_x(\rho u) &= 0 \\ \partial_t(\rho u) + \partial_x(\rho u^2) &= 0 \end{cases} \qquad (x,t) \in \mathbb{R} \times (0,+\infty)$$

with the initial condition

$$\begin{cases} \rho(x,0) &= \rho^{in}(x) \\ u(x,0) &= u^{in}(x) \end{cases}$$

where $\rho(x,t)$ is density field and $u(x,t)$ velocity field. The first equation is for the conservation of mass and the second one for the conservation of momentum.

Limits and Continuity

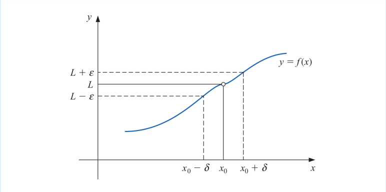
Definition

A function f defined on a set X of real number has the **limit** *L at x_0, written*

$$\lim_{x \to x_0} f(x) = L$$

if, given any real number $\varepsilon > 0$, there exists a real number $\delta > 0$ such that

$$|f(x) - L| < \varepsilon, \quad \textit{whenever} \quad x \in X \quad \textit{and} \quad 0 < |x - x_0| < \delta$$



Limits and Continuity (Cont.)

Definition

Let f be a function defined on a set X of real numbers and $x_0 \in X$. Then f is **continuous** *at x_0 if*

$$\lim_{x \to x_0} f(x) = f(x_0)$$

The function f is **continuous on the set** *X if it is continuous at each number in X.*

Definition

Let $\{x_n\}_{n=1}^{\infty}$ be a infinity of real number. This sequence has the **limit** *x (***converges to** *x) if, for any $\varepsilon > 0$, there exists a positive integer $N(\varepsilon)$ such that $|x_n - x| < \varepsilon$, whenever $n > N(\varepsilon)$. The notation*

$$\lim_{n\to\infty} x_n = x \quad \text{or} \quad x_n \to x \quad \text{as} \quad n \to \infty$$

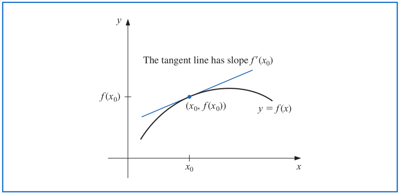
Differentiability

Definition

Let f be a function defined on a open interval containing x_0. The function f is **differentiable** *at x_0 if*

$$f'(x_0) = \lim_{x \to x_0} \frac{f(x) - f(x_0)}{x - x_0}$$

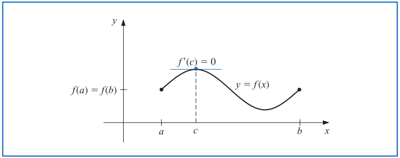
exists. The number $f'(x_0)$ is called the **derivative** *of f at x_0.*



Differentiability (Cont.)

Theorem (Rolle's Theorem)

Suppose $f \in C([a,b])$ and f is differentiable on (a,b). If $f(a) = f(b)$, then a number c in (a,b) exists with $f'(c) = 0$.

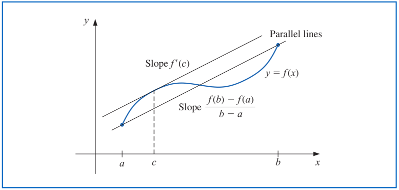


Differentiability (Cont.)

Theorem (Mean Value Theorem)

If $f \in C([a,b])$ and f is differentiable on (a,b), then a number c in (a,b) exists with

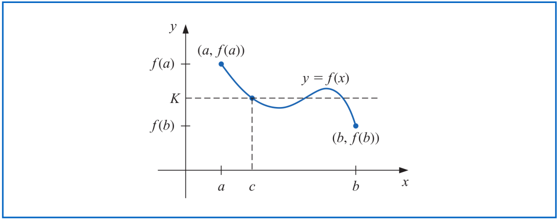
$$f'(c) = \frac{f(b) - f(a)}{b - a}$$



Differentiability (Cont.)

Theorem (Intermediate Value Theorem)

If $f \in C([a,b])$ and K is any number between $f(a)$ and $f(b)$. then there exists a number c in (a,b) such that $f(c) = K$



Exercise:

1.1/ Show that the following equations have at least one solution in the given intervals

a. $xcosx - 2x^2 + 3x - 1 = 0$, $[0.2, 0.3]$ and $[1.2, 1.3]$

b. $(x-2)^2 - lnx = 0$, $[1, 2]$ and $[e, 4]$

c. $2xcos(2x) - (x-2)^2 = 0$, $[2, 3]$ and $[3, 4]$

d. $x - (lnx)^x = 0$, $[4, 5]$

1.2/ Show that $f'(x) = 0$ at least once in the given intervals a. $f(x) = 1 - e^x + (e-1)\sin(\frac{\pi}{2}x)$, $[0, 1]$

b. $f(x) = (x-1)\tan x + x\sin \pi x$, $[0, 1]$

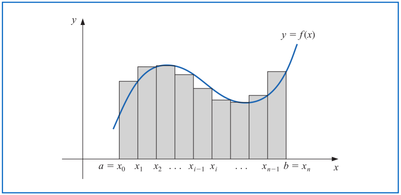
Integration

Definition (Riemann Integral)

The **Riemann integral** *of the function* f *on the interval* $[a, b]$ *is the following limit, provided it exists:*

$$\int_a^b f(x)dx = \lim_{\max \Delta x_i \to 0} \sum_{i=1}^n f(z_i)\Delta x_i$$

where the numbers $x_0, x_1, \cdots, x_n$ *satisfy* $a = x_0 \leq x_1 \leq \cdots \leq x_n = b$, *where* $x_i = x_i - x_{i-1}$, *for each* $i = 1, 2, ..., n$, *and* z_i *is arbitrarily chosen in the interval* $[x_{i-1}, x_i]$.



Taylor Polynomials

Theorem (Taylor's Theorem)

Suppose $f \in C^n([a,b])$, that $f^{(n+1)}$ exists on $[a,b]$, and $x_0 \in [a,b]$. For every $x \in [a,b]$, there exists a number $\xi(x)$ between x_0 and x with

$$f(x) = P_n(x) + R_n(x)$$

where

$$P_n = f(x_0) + f'(x_0)(x - x_0) + \frac{f''(x_0)}{2!}(x - x_0)^2 + \cdots + \frac{f^{(n)}(x_0)}{n!}(x - x_0)^n$$

and

$$R_n(x) = \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)^{n+1}$$

Taylor Polynomials

Example

Let $f(x) = cosx$ *and* $x_0 = 0$. *Determine*

(a) *the second Taylor polynomial for* f *about* x_0 ; *and*

(b) *the third Taylor polynomial for* f *about* x_0 .

Exercise:

1.3/ Let $f(x) = x^3$

a. Find the second Taylor polynomial $P_2(x)$ about $x_0 = 0$

b. Find $R_2(0.5)$. Estimate error when using $P_2(0.5)$ to approximate $f(0.5)$

1.4/ Find the third Taylor polynomial $P_3(x)$ for the function $f(x) = \sqrt{x+1}$ about $x_0 = 0$. Approximate $\sqrt{0.5}, \sqrt{1.5}$ using $P_3(x)$.

1.5/ Let $f(x) = 2x\cos(2x) - (x-2)^2$ and $x_0 = 0$

a. Find the third Taylor polynomial $P_3(x)$ and use it to approximate $f(0.4)$.

b. Use the error formula in Taylor's Theorem to find an upper bound for the error $|f(0.4) - P_3(0.4)|$.

1.6/ Using a Taylor polynomial about $\pi/4$ to approximate $\cos 42^o$ to an accuracy of 10^{-6}.

Absolute Error and Relative Error

Definition

Suppose that p^* is an approximation to p.

$$\textbf{absolute error} = |p - p^*|, \qquad \textbf{relative error} = \frac{|p - p^*|}{p}$$

$$\textbf{relative error} = \frac{|current\ approximation - previous\ approximation|}{current\ approximation}$$

Definition (Truncation Error)

Difference between true result and result produced by given algorithm

Exercise:

1.7/Compute the absolute error and relative error in approximations of p and p^*.

a. $p = \pi,\ p^* = 22/7$

b. $p = e,\ p^* = 2.718$

c. $p = e^10,\ p^* = 22000$

d. $p = 8!,\ p^* = 39900$

Exercise:

1.8/ Suppose p^* must approximate p with relative error at most 10^{-3}. Find the largest interval in which p^* must lie for each value of p

a. $p = 150$

b. $p = 900$

c. $p = 1500$

d. $p = 90$

1.9/ Suppose p^* must approximate p with relative error at most 10^{-4}. Find the largest interval in which p^* must lie for each value of p

a. $p = \pi$

b. $p = \sqrt{2}$

c. $p = e$

d. $p = \sqrt[3]{7}$

Exercise (at home):

1.10/ Use the Intermediate Value Theorem and Roll's Theorem to show that the graph of $f(x) = x^3 + 2x + k$ crosses the x-axis exactly once, regardless of the value of the constant k.

1.11/Prove

Theorem (the Generalized Roll's Theorem)

Suppose $f \in C([a,b])$ is n times differentiable on (a,b). If $f(x) = 0$ at $n+1$ distinct numbers $a \le x_0 < x_1 < \ldots < x_n \le b$, then a number c in (x_0, x_n) and hence in (a,b) exists with $f^{(n)}(c) = 0$.

We consider the model of the growth of a population. The population $N(t)$ at time t satisfies

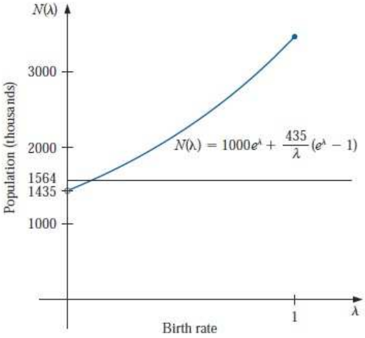
$$\frac{dN(t)}{dt} = \lambda N(t) + \upsilon$$

where λ is constant birth rate and υ is constant immigration rate. The solution is

$$N(t) = N_0 e^{\lambda t} + \frac{\upsilon}{\lambda}(e^{\lambda t} - 1)$$

Suppose initial population $N(0) = 1,000,000$, immigration rate $435,000$, population after one year $N(1) = 1,564,000$. Let determine the birth rate of this population λ.
We have

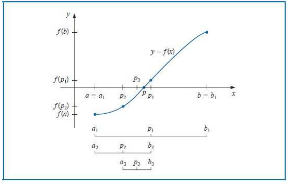
$$1,564,000 = 1,000,000e^{\lambda} + \frac{435,000}{\lambda}(e^{\lambda} - 1)$$



Definition

Suppose f is a continuous function on $[a, b]$ and $f(a).f(b) < 0$, then it exists $p \in (a, b)$ that $f(p) = 0$ (by Intermediate Value Theorem). Bisection is the method calling for a repeated halving of subintervals $[a, b]$.

Description



Set $a_1 = a$ and $b_1 = b$ and let $p_1 = a_1 + \frac{b_1 - a_1}{2}$

- If $f(p_1) = 0$, then $p = p_1$
- If $f(p_1) \neq 0$, then
  -If $f(p_1).f(a_1) > 0$, set $a_2 = p_1,\ b_2 = b_1$
  -If $f(p_1).f(a_1) < 0$, set $a_2 = a_1,\ b_2 = p_1$

Repeat this process to the interval $[a_2, b_2]$.

Algorithm of Bisection

INPUT: function f, endpoints a, b, tolerance TOL, maximum number of iterations N_0
OUTPUT: approximation solution p or message of failure.
Step 1: Set $i = 1$, $FA = f(a)$.
Step 2: While $i \leq N_0$
-Step 2.1: Set $p = a + \frac{b-a}{2}$, $FP = f(p)$
-Step 2.2: If $FP = 0$ or $(b-a)/2 < TOL$
then OUTPUT(p) and STOP
-Step 2.3: Set $i = i + 1$.
-Step 2.4: If $FA.FP > 0$ then set $a = p$, $FA = FP$, else $b = p$.
Step 3: OUTPUT (Method fail after N_0 iterations), STOP.
NOTE: We should use $sign(FA).sign(FP) > 0$ instead of $FA.FP > 0$ to avoid overflow.

Stopping criteria

$$|p_N - p_{N-1}| < \varepsilon \tag{1}$$

$$\frac{|p_N - p_{N-1}|}{|p_N|} < \varepsilon, \qquad p_N \neq 0 \tag{2}$$

$$|f(p_N)| < \varepsilon \tag{3}$$

Example

Find root of $f(x) = x^3 + 4x^2 - 10 = 0$ in $[1, 2]$.
$f(1) = -5$, $f(2) = 14$.

n	a_n	b_n	p_n	$f(p_n)$
1	1.0	2.0	1.5	2.375
2	1.0	1.5	1.25	−1.79687
3	1.25	1.5	1.375	0.16211
4	1.25	1.375	1.3125	−0.84839
5	1.3125	1.375	1.34375	−0.35098
6	1.34375	1.375	1.359375	−0.09641
7	1.359375	1.375	1.3671875	0.03236
8	1.359375	1.3671875	1.36328125	−0.03215
9	1.36328125	1.3671875	1.365234375	0.000072
10	1.36328125	1.365234375	1.364257813	−0.01605
11	1.364257813	1.365234375	1.364746094	−0.00799
12	1.364746094	1.365234375	1.364990235	−0.00396
13	1.364990235	1.365234375	1.365112305	−0.00194

Theorem (2.1)

Suppose $f \in C[a,b]$ *and* $f(a).f(b) < 0$. *The Bisection method generates a sequence* $\{p_n\}_{n=1}^{\infty}$ *approximating a zero* p *of* f *with*

$$|p_n - p| \leq \frac{b-a}{2^n}, \quad \text{when} \quad n \geq 1.$$

Exercise

2.1/ Use Bisection method to find approximation solutions with $TOL = 10^{-5}$ for the following problems

a. $x - 2^{-x} = 0, \ x \in [0, 1]$

b. $e^x - x^2 + 3x - 2 = 0, \ x \in [0, 1]$

c. $2x\cos(2x) - (x+1)^2 = 0 \ x \in [-3, -2]$ and $x \in [-1, 0]$

d. $x\cos(x) - 2x^2 + 3x - 1 = 0 \ x \in [0.2, 0.3]$ and $x \in [1.2, 1.3]$

2.2/ a. Plot the graphs of $y = e^x - 2$ and $y = \cos(e^x - 2)$.

b. Use Bisection method to find approximation solutions of $e^x - 2 = \cos(e^x - 2)$ with relative error less than 10^{-5} in $[0.5, 1.5]$.

Definition

The number p is a **fixed point** *for a given function g if $g(p) = p$.*

Note: Root-finding problem and fixed-point problem are equivalent.

$$g(x) = x - f(x)$$

Example: Determine fixed points of the function $g(x) = x^2 - 2$

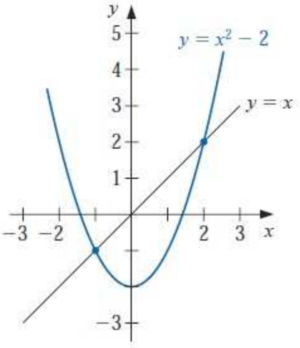
Example

Determine fixed points of the function $g(x) = x^2 - 2$.

Solution:

$g(p) = p^2 - 2 = p \iff p^2 - p - 2 = (p+1)(p-2) = 0$

$\Rightarrow p = -1$ or $p = 2$



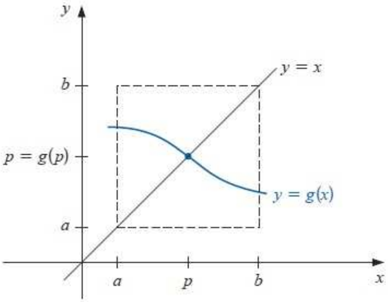
Theorem (2.2)

(i) Existence *If* $g \in C[a,b]$ *and* $g(x) \in [a,b], \forall x \in [a,b]$, *then* g *has at least one fixed point in* $[a,b]$.

(ii) Uniqueness *If, in addition,* $g'(x)$ *exists on* (a,b) *and*

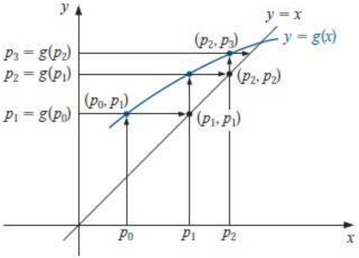
$$|g'(x)| \leq k < 1, \quad \forall x \in (a,b)$$

then there is exactly one fixed point $p \in [a,b]$



Fixed-point iteration

Let g be continuous, p_0 be an initial approximation. Put $p_n = g(p_{n-1}), \forall n \geq 1$. If $p_n \to p$, then p= g(p)



Algorithm of Fixed-point iteration

INPUT: function g, initial approximation p_0, tolerance TOL, maximum number of iterations N_0
OUTPUT: approximation solution p or message of failure.
Step 1: Set $i = 1$.
Step 2: While $i \leq N_0$
-Step 2.1: Set $p = g(p_0)$
-Step 2.2: If $|p - p_0| < TOL$
then OUTPUT(p) and STOP
-Step 2.3: Set $i = i + 1$.
-Step 2.4: Set $p_0 = p$.
Step 3: OUTPUT (Method fail after N_0 iterations), STOP.

Theorem (2.3)

Let $g \in C[a,b]$ *and* $g(x) \in [a,b], \forall x \in [a,b]$. *Suppose* $g'(x)$ *exists on* (a,b) *and*

$$|g'(x)| \leq k < 1, \quad \forall x \in (a,b)$$

then $\forall p_0 \in [a,b]$, *the sequence defined by* $p_n = g(p_{n-1}), \quad n \geq 1$ *converges to the unique fixed point* $p \in [a,b]$.

Corllory (2.3)

Let g *satisfies the hypotheses of Theorem 2.3, then*

$$|p_n - p| \leq k^n \max\{p_0 - a, b - p_0\}$$

and

$$|p_n - p| \leq \frac{k^n}{1-k}|p_1 - p_0|, \quad \forall n \geq 1.$$

Example

Find the solution of the equation $x^3 + 4x^2 - 10 = 0$ in $[1, 2]$.

a/ $x = g_1(x) = x - x^3 - 4x^2 + 10$ b/ $x = g_2(x) = \left(\frac{10}{x} - 4x\right)^{1/2}$

c/ $x = g_3(x) = \frac{1}{2}\left(10 - x^3\right)^{1/2}$ d/ $x = g_4(x) = \left(\frac{10}{4+x}\right)^{1/2}$

e/ $x = g_5(x) = x - \frac{x^3+4x^2-10}{3x^2+8x}$

n	(a)	(b)	(c)	(d)	(e)
0	1.5	1.5	1.5	1.5	1.5
1	−0.875	0.8165	1.286953768	1.348399725	1.373333333
2	6.732	2.9969	1.402540804	1.367376372	1.365262015
3	−469.7	$(-8.65)^{1/2}$	1.345458374	1.364957015	1.365230014
4	1.03×10^8		1.375170253	1.365264748	1.365230013
5			1.360094193	1.365225594	
6			1.367846968	1.365230576	
7			1.363887004	1.365229942	
8			1.365916734	1.365230022	
9			1.364878217	1.365230012	
10			1.365410062	1.365230014	
15			1.365223680	1.365230013	
20			1.365230236		
25			1.365230006		
30			1.365230013		

Exercise

2.3/ The following four methods are proposed to compute $7^{1/5}$. Rank them in order, based on their apparent speed of convergence, $p_0 = 1$.

a. $p_n = p_{n-1}\left(1 + \frac{7-p_{n-1}^5}{p_{n-1}^2}\right)^3$

b. $p_n = p_{n-1} - \frac{p_{n-1}^5-7}{p_{n-1}^2}$

c. $p_n = p_{n-1} - \frac{p_{n-1}^5-7}{5p_{n-1}^4}$

d. $p_n = p_{n-1} - \frac{p_{n-1}^5-7}{12}$.

2.4/ $f(x) = x^4 - 3x^2 - 3 = 0,\ x \in [1, 2]$, use a fixed point iteration method to determine a solution accurate to with thin 10^{-2}, $p_0 = 1$.

Exercise (Home)

2.5/ Let $f(x) = (x-1)^{10}, p = 1$ and $p_n = 1 + 1/n$. Show that $|f(p_n)| < 10^{-3}, \quad n > 1$ but $|p - p_n| < 10^{-3}$ requires that $n > 1000$.

2.6/ The function defined by $f(x) = \sin(\pi x)$ has solutions at every integer. Show that when $a \in (-1, 0), b \in (2, 3)$, the Bisection method converges to

a. 0, if $a + b < 2$ b. 2, if $a + b > 2$ c. 1, if $a + b = 2$

2.7/ a. Show that for $A > 0$, then the sequence

$$x_n = \frac{1}{2}x_{n-1} + \frac{A}{2x_{n-1}}, \qquad \forall n \geq 1,$$

converges to $\sqrt{A}$ whenever $x_0 > 0$.

b. What happens if $x_0 < 0$.

Let consider the population of Vietnam:

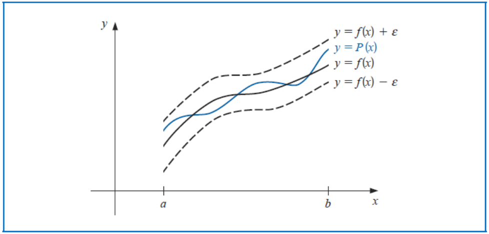
Year	1980	1985	1990	1995	2000	2005
Population (10^3)	53722	59872	66016	71995	77635	83106

What is population of Vietnam in 1997? 2015?

Theorem (3.1 (Weierstrass Approximation))

Let $f \in C[a, b]$. For each $\varepsilon > 0$, there exist a polynomial $P(x)$ such that

$$|f(x) - P(x)| < \varepsilon \qquad \forall x \in [a, b]$$

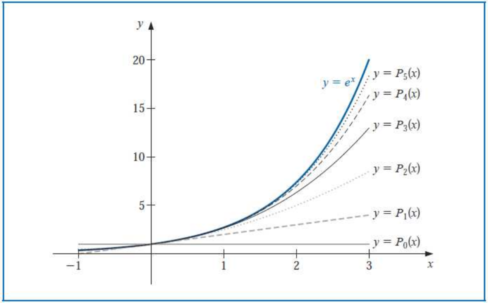


Example

Recall Taylor polynomial for $f(x) = e^x$ about $x_0 = 0$

$P_0(x) = 1, P_1(x) = 1+x, P_2(x) = 1+x+\frac{x^2}{2}, P_3(x) = 1+x+\frac{x^2}{2}+\frac{x^3}{6}$

$P_4(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24}, P_5(x) = 1 + x + \frac{x^2}{2} + \frac{x^3}{6} + \frac{x^4}{24} + \frac{x^5}{120}$



Example

Taylor polynomial for $f(x) = \frac{1}{x}$ about $x_0 = 1$

$$f^{(k)}(x) = (-1)^k.k!.x^{-k-1},$$

$$P_n(x) = \sum_{k=0}^{n} \frac{f^{(k)}(1)}{k!}(x-1)^k = \sum_{k=0}^{n} (-1)^k (x-1)^k$$

n	0	1	2	3	4	5	6	7
$P_n(3)$	1	-1	3	-5	11	-21	43	-85

Lagrange interpolating polynomials

Give two points $(x_0, y_0), (x_1, y_1)$. We define the functions:

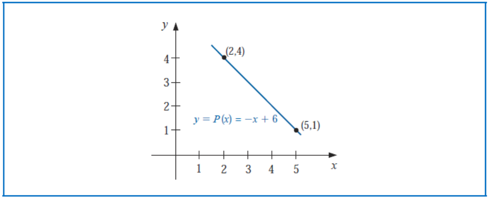
$$L_0(x) = \frac{x - x_1}{x_0 - x_1} \qquad \text{and} \qquad L_1(x) = \frac{x - x_0}{x_1 - x_0}$$

The **linear Lagrange interpolating polynomial** through (x_0, y_0) and (x_1, y_1) is

$$P(x) = L_0(x)y_0 + L_1(x)y_1 = \frac{x - x_1}{x_0 - x_1}y_0 + \frac{x - x_0}{x_1 - x_0}y_1$$

Example

Find the linear Lagrange interpolating polynomial that passes through the points $(2, 4)$ and $(5, 1)$.



Lagrange interpolating polynomials

For each $k = 0, 1, ..., n$, we define a function

$$L_{n,k}(x) = \frac{(x - x_0)...(x - x_{k-1})(x - x_{k+1})...(x - x_n)}{(x_k - x_0)...(x_k - x_{k-1})(x_k - x_{k+1})...(x_k - x_n)}$$

that

$$L_{n,k}(x_i) = \begin{cases} 0 & , i \neq k \\ 1 & , i = k \end{cases}$$

Theorem (3.2)

If $x_0, x_1, ..., x_n$ *are* $n+1$ *distinct numbers and a function* f *that* $f(x_k)$, $k = 0, ..., n$ *are given.*
Then there exists a unique polynomial $P(x)$ *of degree at most* n *such that* $P(x_k) = f(x_k)$ *and*

$$P(x) = f(x_0)L_{n,0}(x) + ... + f(x_n)L_{n,n}(x) = \sum_{k=0}^{n} f(x_k)L_{n,k}(x)$$

where

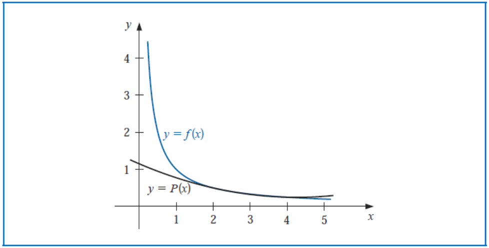
$$L_{n,k}(x) = \frac{(x-x_0)...(x-x_{k-1})(x-x_{k+1})...(x-x_n)}{(x_k-x_0)...(x_k-x_{k-1})(x_k-x_{k+1})...(x_k-x_n)}$$

Example

- Give $x_0 = 2$, $x_1 = 2.75$, $x_2 = 4$. Find the second Lagrange interpolating polynomial for $f(x) = 1/x$.
- Use this polynomial to approximate $f(x) = 1/3$.

$$P(x) = \frac{1}{22}x^2 - \frac{35}{88}x + \frac{49}{44}$$

$$P(3) = \frac{29}{88} \approx 0.32055$$



Theorem (3.3)

If $x_0, x_1, ..., x_n$ are $n+1$ distinct numbers in the interval $[a, b]$ and $f \in C^{n+1}[a, b]$.
Then for $x \in [a, b]$, there exists a number $\xi(x) \in (a, b)$ that

$$f(x) = P_n(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x - x_0)(x - x_1)...(x - x_n)$$

where

$$P_n(x) = \sum_{k=0}^{n} f(x_k) L_{n,k}(x)$$

$$L_{n,k}(x) = \prod_{i=0, i \neq k}^{n} \frac{(x - x_i)}{(x_k - x_i)}$$

if $x = x_k$, for any $k = 0, 1, ..., n$ then $f(x_k) = P(x_k)$.
If $x \neq x_k$, for all $k = 0, 1, ..., n$, we define the function g for t in $[a, b]$ by

$$g(t) = f(t) - P(t) - [f(x) - P(x)]\frac{(t - x_0)(t - x_1)...(t - x_n)}{(x - x_0)(x - x_1)...(x - x_n)}$$
$$= f(t) - P(t) - [f(x) - P(x)]\prod_{i=0}^{n}\frac{(t - x_i)}{(x - x_i)}$$

$t = x, x_0, ..., x_n$ then $g(x) = 0$, $g(x_k) = 0$ $k = 0, ..., n$.
Thus $g \in C^{n+1}[a, b]$, and g is zero at the $n + 2$ distinct numbers $x, x_0, x_1, ..., x_n$. By Generalized Rolle's Theorem 1.10, there exists a number $\xi \in (a, b)$ for which $g^{(n+1)}(\xi) = 0$

$$0 = g^{(n+1)}(\xi) = f^{(n+1)}(\xi) - P^{(n+1)}(\xi) - [f(x) - P(x)]\frac{d^{n+1}}{dt^{n+1}}\left[\prod_{i=0}^{n}\frac{(t-x_i)}{(x-x_i)}\right]_{t=\xi}$$

with $\frac{d^{n+1}}{dt^{n+1}}\left[\prod_{i=0}^{n}\frac{(t-x_i)}{(x-x_i)}\right] = \frac{(n+1)!}{\prod_{i=0}^{n}(x-x_i)}$

then

$$0 = f^{(n+1)}(\xi) - 0 - [f(x) - P(x)]\frac{(n+1)!}{\prod_{i=0}^{n}(x-x_i)}$$

Exercise

3.1/ Let $x_0 = 0, x_1 = 0.6, x_2 = 0.9$. Find $L_{1,0}, L_{1,1}$ and $L_{2,0}, L_{2,1}, L_{2,2}$ to approximate $f(0.45)$ and find absolute error following function:
a/ $\cos(x)$
b/ $\sqrt{(1+x)}$
c/ $\ln(x+1)$
d/ $\tan(x)$ 3.2/ Let $x_0 = 1, x_1 = 1.25, x_2 = 1.6$. Find $L_{1,0}, L_{1,1}$ and $L_{2,0}, L_{2,1}, L_{2,2}$ to approximate $f(1.4)$ and find absolute error following function:
a/ $\sin(\pi x)$
b/ $\sqrt[3]{(x-1)}$
c/ $log_{10}(3x-1)$
d/ $e^{2x} - x$.

We would like to determine the length of the curve given by $f(x) = \sin(x)$ from 0 to 10. From the caculus, this length is

$$L = \int_0^{10} \sqrt{1 + (f'(x))^2} dx = \int_0^{10} \sqrt{1 + \cos^2(x)} dx$$

How to compute the integration????

The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h) - f(x_0)}{h}$$

When h is small, we can write

$$f'(x_0) \simeq \frac{f(x_0+h) - f(x_0)}{h}$$

In this approximation, we can not dertimine the the error between the approximated value and exact value.

To appromate $f'(x_0)$, we suppose first that $x_0 \in (a, b)$, where $f \in C^2([a, b])$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$. Using Taylor serries, there exists $\xi \in (x_0, x_1)$ such that

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{h^2}{2} f''(\xi)$$

Thus

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi)$$

Since $f \in C^2([a, b])$, there exists positive constant M such that $|f''(x)| < M$, thus $|\frac{h}{2} f''(\xi)| < Mh/2$. We can rewrite

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} + 0(h)$$

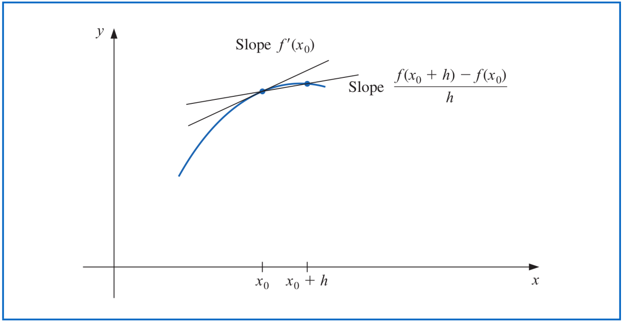
For h is small, $\frac{f(x_0+h)-f(x_0)}{h}$ is used to appromate the value $f'(x_0)$ with an errror $0(h)$.
For $h > 0$, we can write

$$f'(x_0) \simeq \frac{f(x_0+h)-f(x_0)}{h} \qquad \text{forward-difference formula}$$

$$f'(x_0) \simeq \frac{f(x_0)-f(x_0-h)}{h} \qquad \text{backward-difference formula}$$

Example:

Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.



Hình: Forward difference

Three endpoint formula

Given three 3 point $x_0, x_0 + h, x_0 + 2h \in (a, b)$. We would like to appromate $f'(x_0)$. Using Taylor serries, there exist $\xi_1 \in (x_0, x_0 + h)$ and $\xi_2 \in (x_0, x_0 + 2h)$, such that

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(\xi_1)$$

and

$$f(x_0 + 2h) = f(x_0) + 2hf'(x_0) + \frac{(2h)^2}{2} f''(x_0) + \frac{(2h)^3}{6} f'''(\xi_2)$$

From two approximation, we have

$$f(x_0+2h)-4f(x_0+h) = -3f(x_0)-2hf'(x_0)+h^3\left(\frac{8}{6} f'''(\xi_2)-\frac{4}{6} f'''(\xi_1)\right)$$

Three endpoint formula

Then

$$f'(x_0) = \frac{-3f(x_0) - 4f(x_0+h) - f(x_0+2h)}{2h} + h^2(\frac{4}{6}f'''(\xi_2) - \frac{2}{6}f'''(\xi_1))$$

We supposr that $f \in C^3([a,b])$, there exist constant $M > 0$ such that

$$h^2(\frac{4}{6}f'''(\xi_2) - \frac{2}{6}f'''(\xi_1)) \leq Mh^2$$

Then

$$f'(x_0) = \frac{-3f(x_0) - 4f(x_0+h) - f(x_0+2h)}{2h} + 0(h^2)$$

Then, three endpoint formula is

$$f'(x_0) = \frac{-3f(x_0) - 4f(x_0+h) - f(x_0+2h)}{2h}$$

Three midpoint formula

Given three 3 point $x_0 - h, x_0, x_0 + h \in (a, b)$. We would like to appromate $f'(x_0)$. Using Taylor serries, there exist $\xi_1 \in (x_0, x_0 + h)$ and $\xi_2 \in (x_0 - h, x_0)$, such that

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{6}f'''(\xi_1)$$

and

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{6}f'''(\xi_2)$$

From two approximation, we have

$$f(x_0 + h) - f(x_0 - h) = 2hf'(x_0) + h^3(f'''(\xi_2) + f'''(\xi_1))$$

Three midpoint formula

Then

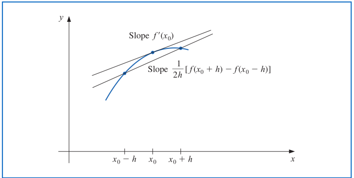
$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - h^2(f'''(\xi_2) + f'''(\xi_1))$$

We supposr that $f \in C^3([a,b])$, there exist constant $M > 0$ such that

$$h^2(f'''(\xi_2) + f'''(\xi_1)) \leq Mh^2$$

Then three midpoint formula

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} + 0(h^2)$$



Example:

Values for $f(x) = xe^x$ are given in Table (2). Use all the applicable forward difference, backward difference, three-point formulas to approximate $f'(2.0)$ and determine bounds for the approximation errors

Bảng: Value of the function $f(x) = xe^x$

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Second derivative midpoint formula

To appromate $f''(x_0)$, we suppose first that $x_0 - h, x_0, x_0 + h \in (a, b)$, where $f \in C^4([a, b])$. Using Taylor serries, there exists $\xi_1 \in (x_0, x_0 + h)$, $\xi_2 \in (x_0 - h, x_0)$ such that

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(\xi_1)$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f'''(x_0) + \frac{h^4}{24} f^{(4)}(\xi_2)$$

Thus

$$f(x_0 + h) - f(x_0 - h) = h^2 f''(x_0) + \frac{h^4}{24}(f^{(4)}(\xi_1) + f^{(4)}(\xi_2))$$

Second derivative midpoint formula

We can rewrite that

$$f''(x_0) = \frac{f(x_0+h) - f(x_0-h)}{h^2} - \frac{h^2}{24}(f^{(4)}(\xi_1) + f^{(4)}(\xi_2))$$

Since $f \in C^4([a,b])$ there exist constant $M > 0$ such that

$$|-\frac{h^4}{24}(f^{(4)}(\xi_1) + f^{(4)}(\xi_2))| \leq Mh^2$$

Then second derivative midpoint formula is

$$f''(x_0) = \frac{f(x_0+h) - f(x_0-h)}{h^2} + 0(h^2)$$

Example:

Use the second derivative formula to approximate f (2.0) with value of f at following table

Bảng: Value of the function $f(x) = xe^x$

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Exercises

1. Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables

x	$f(x)$	$f'(x)$
0.5	0.4794	
0.6	0.5646	
0.7	0.6442	

2. The data in Exercise 1 were taken from the function $f(x) = \sin x$. Compute the actual errors in Exercise 1, and find error bounds using the error formulas.

Exercises

3. Use the most accurate three-point formula to determine each missing entry in the following tables.

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

4. The data in Exercise 3 were taken from the function $f(x) = e^{2x}$. Compute the actual errors in Exercise 3, and find error bounds using the error formulas.

Exercises

5. Let $f(x) = 3xe^x - \cos x$. Use the following data and second derivative midpoint formula to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

x	1.2	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

Compare your results with $f''(1.30)$.

6. Derive an $0(h^4)$ five-point formula to approximate $f'(x_0)$ that uses $f(x_0 - 2h)$, $f(x_0 - h)$, $f(x_0)$, $f(x_0 + h)$, and $f(x_0 + 2h)$.

7. Derive an $0(h^4)$ five-point formula to approximate $f''(x_0)$ that uses $f(x_0 - 2h)$, $f(x_0 - h)$, $f(x_0)$, $f(x_0 + h)$, and $f(x_0 + 2h)$

Introduction

Goal: Determine $\int_a^b f(x)dx$ for f at least continuous on $[a, b]$ with a, b real.

Solution: Approximate f by a Lagrange polynomial

$$f \sim P$$

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

Quadrature formula

Definition

We call quadrature formula $I_n = \sum_{k=0}^{n} a_k f(x_k)$ *that approximate*

$I = \int_a^b f(x)dx$ *for* a, b *in* $\mathbb{R}$ *and* f *is continuous on* $[a, b]$.

The $(x_k)_{k=0,\cdots,n}$ are called the integration nodes.
The $(a_k)_{k=0,\cdots,n}$ are called the weights

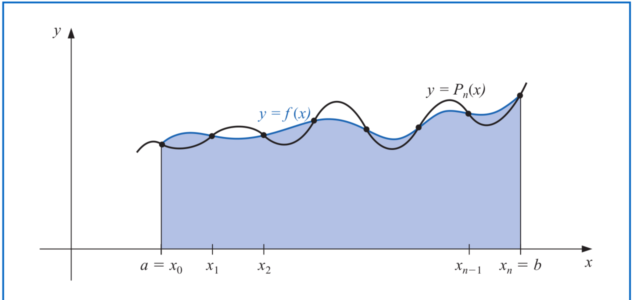
A closed Newton-Cotes Formula

We define the $(x_k)_{k=0,\cdots,n}$ as follows

$$x_k = a + \frac{k}{n}(b-a) \quad \forall k = 0, \cdots, n$$

$$x_0 = a, \qquad x_n = b$$

$$\frac{b-a}{n} \text{ often is denoted by } h$$



A closed Newton-Cotes Formula

Definition

A closed Newton-Cotes approximation of degree n (NC_n) *consists of approximation of* $I = \int_a^b f(x)dx$ *by*

$$I_n = \int_a^b P(x)dx = \sum_{k=0}^{n} a_k f(x_k)$$

where P *is Lagrange polynomial of* f *at* $x_0, \cdots, x_n$.

A closed Newton-Cotes Formula

Proposition

In the closed Newton-Cotes formula, we have

$$a_k = \int_a^b L_k(x)dx$$

where $L_k(x) = \prod_{j=1, j \neq k}^{n} \frac{x - x_j}{x_k - x_j}$

Proof: From definition of Lagrange polynomial P of f, we have

$$P(x) = \sum_{k=1}^{n} f(x_k)L_k(x), \quad \text{where } L_k(x) = \prod_{j=1, j \neq k}^{n} \frac{x - x_j}{x_k - x_j}$$

Then

$$\int^b P(x)dx = \sum^n f(x_k) \int^b L_k(x)dx = \sum^n a_k f(x_k)$$

A closed Newton-Cotes Formula

Theorem

On the interval $[a, b]$*, we assume that* $f \in C^{n+1}([a, b])$*, then*

$$R(f) = \left| \int_a^b f(x)dx - \int_a^b P(x)dx \right| \leq (b-a)^{n+2} \frac{\|f^{(n+1)}\|_\infty}{(n+1)!}$$

where $\|f^{(n+1)}\|_\infty = \sup_{x \in [a,b]} |f^{(n+1)}(x)|$

Proof: From definition of Lagrange polynomial P of f, there exist $\xi_x \in [a, b]$ such that

$$f(x) = P(x) + \prod_{k=0}^{n} \frac{(x - x_k)}{k+1} f^{(n+1)}(\xi)$$

A closed Newton-Cotes Formula

$$R(f) = \left| \int_a^b f(x)dx - \int_a^b P(x)dx \right| \leq \int_a^b |f(x)dx - P(x)|dx$$
$$= \int_a^b \left| \prod_{k=0}^{n} \frac{(x - x_k)}{k+1} f^{(n+1)}(\xi_x) \right| dx$$

Because $x \in [a, b]$ and $x_k \in [a, b]$ for all $k = 0, \cdots, n$, we have

$$|x - x_k| \leq (b - a) \quad \forall k = 0, \cdots, n$$

Since $\xi_x \in [a, b]$ then

$$|f^{(n+1)}(\xi_x)| \leq \sup_{x \in [a,b]} |f^{(n+1)}(x)| = \|f^{(n+1)}\|_\infty$$

$$R(f) \leq (b - a)^{n+1} \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} \int_a^b dx = (b - a)^{n+2} \frac{(\|f^{(n+1)}\|_\infty}{(n+1)!}$$

Trapezoidal Rule (NC_1)

★ n=1 (2 nodes integration), $x_0 = a,\ x_1 = b$.
First, we build Lagrange polynomial at $(x_0, f(x_0))$ and $(x_1, f(x_1))$ i.e $(a, f(a))$ and $(b, f(b))$.

$$P_1(x) = f(x_0)L_0(x) + f(x_1)L_1(x)$$

where

$$L_0(x) = \frac{x - x_1}{x_0 - x_1} = \frac{x - b}{a - b}, \qquad L_1(x) = \frac{x - x_0}{x_1 - x_0} = \frac{x - a}{b - a}$$

This implies

$$I_1(f) = \int_a^b P_1(t)dt = f(a)\int_a^b \frac{t - b}{a - b}dt + f(b)\int_a^b \frac{t - a}{b - a}dt$$

Trapezoidal Rule (NC_1)

It is easy to have

$$\int_a^b \frac{t-b}{a-b}dt = \frac{b-a}{2}, \qquad \int_a^b \frac{t-a}{b-a}dt = \frac{b-a}{2}$$

Then

$$I_1(f) = \frac{b-a}{2}f(a) + \frac{b-a}{2}f(b)$$

Proposition

$$R(f) = \left| \int_a^b f(x)dx - \frac{b-a}{2}(f(a)+f(b)) \right| \leq \frac{(b-a)^2}{2}\|f^{(2)}\|_\infty$$

Remark: *we can prove that* $R(f) \leq \frac{(b-a)^2}{12}\|f^{(2)}\|_\infty$

Simpson's rule (NC_2)

★ $n = 2$ (3 nodes integration), $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$.

$$\begin{aligned} P_2(x) &= f(x_0)L_0(x) + f(x_1)L_1(x) + f(x_2)L_2(x) \\ &= f(a)L_0(x) + f(\frac{a+b}{2})L_1(x) + f(b)L_2(x) \end{aligned}$$

where

$$\begin{aligned} L_0(x) &= \frac{(x - \frac{a+b}{2})(x-b)}{(a - \frac{a+b}{2})(a-b)}, \\ L_1(x) &= \frac{(x-a)(x-b)}{(\frac{a+b}{2} - a)(\frac{a+b}{2} - b)} \\ L_2(x) &= \frac{(x-a)(x - \frac{a+b}{2})}{(b-a)(b - \frac{a+b}{2})} \end{aligned}$$

Simpson's rule (NC_2)

$$\int_a^b P(x)dx = f(a)\int_a^b L_0(t)dt + f(\frac{a+b}{2})\int_a^b L_1(t)dt + f(b)\int_a^b L_2(t)dt$$

$$\int_a^b L_0(t)dt = \frac{b-a}{6}$$

$$\int_a^b L_1(t)dt = \frac{4(b-a)}{6}$$

$$\int_a^b L_2(t)dt = \frac{b-a}{6}$$

Then Simpson's rule is

$$I_2(f) = \frac{b-a}{6}\left(f(a) + 4f(\frac{a+b}{2}) + f(b)\right)$$

Simpson's rule (NC_2)

Proposition

If $f \in C^3([a,b])$ *then*

$$\left| \int_a^b f(x)dx - I_2(f) \right| \leq \frac{(b-a)^4}{6} \| f^{(3)} \|_\infty$$

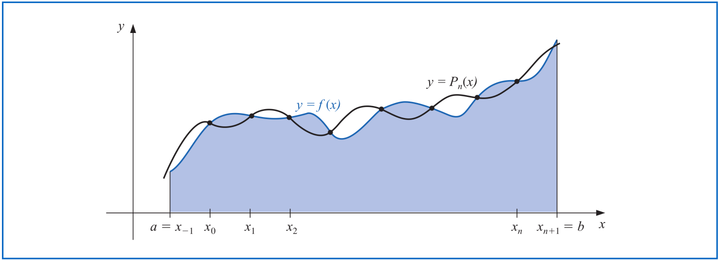
Example

Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x)dx$ when $f(x)$ is

- $f(x) = x^2$
- $f(x) = \sin(x)$
- $f(x) = \frac{1}{1+x}$

A open Newton-Cotes formula

We use the nodes: $x_k = x_0 + kh$ for all $k = 0, \cdots, n$, where $h = \frac{b-a}{n+2}$, and $x_0 = a + h$, $x_n = b - h$



A open Newton-Cotes formula

Definition

A open Newton-Cotes approximation of degree n (NC_n) consists of approximation of $I = \int_a^b f(x)dx$ by

$$I_n = \int_a^b P(x)dx = \sum_{k=0}^{n} a_k f(x_k)$$

where P is Lagrange polynomial of f at $x_0, \cdots, x_n$.

Proposition

In the open Newton-Cotes formula, we have

$$a_k = \int_a^b L_k(x)dx, \quad \text{where } L_k(x) = \prod_{j=1, j\neq k}^{n} \frac{x - x_j}{x_k - x_j}$$

A open Newton-Cotes formula

Theorem

On the interval $[a, b]$, *we assume that* $f \in C^{n+1}([a, b])$, *then*

$$R(f) = \left| \int_a^b f(x)dx - \int_a^b P(x)dx \right| \leq (b-a)^{n+2} \frac{\|f^{(n+1)}\|_\infty}{(n+1)!}$$

where $\|f^{(n+1)}\|_\infty = \sup_{x \in [a,b]} |f^{(n+1)}(x)|$

Midpoint rule

★ n=0 (Midpoint rule). We take 1 node $x_0 = \frac{a+b}{2}$.

$$P_0(x) = f(\frac{a+b}{2})L_0(x) \quad \forall x \in [a,b]$$

This implies

$$\int_a^b P_0(x)dx = \int_a^b f(\frac{a+b}{2})dx = (b-a)f(\frac{a+b}{2})$$

Proposition

If $f \in C^2([a,b])$, then

$$R_0(f) = \left| \int_a^b f(x)dx - (b-a)f(\frac{a+b}{2}) \right| \le (b-a)^2 \|f^{(2)}\|_\infty$$

Midpoint rule

Theorem (Error estimate for the midpoint rule)

If $f \in C^2([a,b])$ *then*

$$\left|\int_a^b f(x)dx - (b-a)f(\frac{a+b}{2})\right| \leq \frac{\|f^{(2)}\|}{24}(b-a)^3$$

Proof: When $f \in C^2([a,b])$, then, for all $t \in (a,b)$, there exist $\xi \in (t, \frac{a+b}{2})$ such that

$$f(t) = f(\frac{a+b}{2}) + (t - \frac{a+b}{2})f'(\frac{a+b}{2}) + \frac{1}{2}(t - \frac{a+b}{2})^2 f''(\xi)$$

Integrating over $[a,b]$, we have

$$\int_a^b f(t)dt = \int_a^b f(\frac{a+b}{2})dt + \int_a^b (t - \frac{a+b}{2})f'(\frac{a+b}{2})dt + \int_a^b \frac{1}{2}(t - \frac{a+b}{2}$$

Midpoint rule

Integrating over $[a, b]$, we have

$$\int_a^b f(t)dt = \int_a^b f(\frac{a+b}{2})dt + \int_a^b (t - \frac{a+b}{2})f'(\frac{a+b}{2})dt + \int_a^b \frac{1}{2}(t - \frac{a+b}{2})^2 f''(\xi)dt = (b-a)f(\frac{a+b}{2}) + 0 + \frac{1}{2}\int_a^b (t - \frac{a+b}{2})^2 f''(\xi)dt$$

Then

$$\int_a^b f(t)dt - (b-a)f(\frac{a+b}{2}) = \frac{1}{2}\int_a^b (t - \frac{a+b}{2})^2 f''(\xi)dt$$

Midpoint rule

We have

$$\left|\int_a^b f(t)dt - (b-a)f(\frac{a+b}{2})\right| \leq \frac{1}{2}\int_a^b (t-\frac{a+b}{2})^2 |f^{(2)}(\xi)|dt$$
$$\leq \frac{1}{2}\int_a^b (t-\frac{a+b}{2})^2 \|f^{(2)}\|_\infty dt$$
$$\leq \frac{\|f^{(2)}\|_\infty}{2}\int_a^b (t-\frac{a+b}{2})^2 dt$$
$$\leq \frac{\|f^{(2)}\|_\infty}{2}\frac{(b-a)^3}{12}$$

Then

$$\left|\int_a^b f(t)dt - (b-a)f(\frac{a+b}{2})\right| \leq \frac{\|f^{(2)}\|_\infty}{24}(b-a)^3$$

Rectangle rule (left)

★ n=0 (Left rule). We take 1 node $x_0 = a$.

$$P_0(x) = f(a)L_0(x) \quad \forall x \in [a, b]$$

This implies

$$\int_a^b P_0(x)dx = \int_a^b f(a)dx = (b-a)f(a)$$

Proposition

If $f \in C^2([a, b])$, then

$$R_0(f) = \left| \int_a^b f(x)dx - (b-a)f(a) \right| \le (b-a)^2 \|f^{(2)}\|_\infty$$

Rectangle rule (right)

★ n=0 (Right rule). We take 1 node $x_0 = b$.

$$P_0(x) = f(b)L_0(x) \quad \forall x \in [a, b]$$

This implies

$$\int_a^b P_0(x)dx = \int_a^b f(b)dx = (b-a)f(b)$$

Proposition

If $f \in C^2([a, b])$, *then*

$$R_0(f) = \left| \int_a^b f(x)dx - (b-a)f(b) \right| \leq (b-a)^2 \|f^{(2)}\|_\infty$$

Exercises

1. Approximate the following integrals using the Trapezoidal rule

a. $\int_0^{0.5} x^4 dx$ b. $\int_1^{1.5} x^2 \ln x dx$

c. $\int_0^{0.35} \frac{1}{x^2-4} dx$ d. $\int_{0.75}^{1.3} \left(\sin^2(x) - 2x\sin(x) + 1\right)$

2. Find a bound for the error in Exercise 1 using the error formula, and compare this to the actual error.

3. Repeat Exercise 1 using Simpson's rule.

4. Repeat Exercise 2 using Simpson's rule and the results of Exercise 3.

5. Repeat Exercise 1 using the Midpoint rule.

Exercises

6. Repeat Exercise 2 using the Midpoint rule and the results of Exercise 5.

7. The Trapezoidal rule applied to $\int_0^2 f(x)dx$ gives the value 4, and Simpson's rule gives the value 2. What is $f(1)$?

8. The Trapezoidal rule applied to $\int_0^2 f(x)dx$ gives the value 5, and the Midpoint rule gives the value 4. What value does Simpson's rule give?

9. Find the degree of precision of the quadrature formula

$$\int_{-1}^{1} f(x)dx = f(\frac{-\sqrt{3}}{3} + f(\frac{\sqrt{3}}{3})$$