Approximation Errors in Computer Arithmetic (Chapters 3 and 4)

Outline:

- Positional notation – binary representation of numbers
  - Computer representation of integers
  - Floating point representation
    IEEE standard for floating point representation
- Truncation errors in floating point representation
  - Chopping and rounding
  - Absolute error and relative error
  - Machine precision
  - Significant digits
- Approximating a function — Taylor series

1 Computer Representation of numbers

1.1 Number Systems (Positional notation)

A base is the number used as the reference for constructing the system.

Base-10: $0, 1, 2, \ldots, 9,$ — decimal
Base-2: 0,1, — binary
Base-8: $0, 1, 2, \ldots, 7,$ — octal
Base-16: $0, 1, 2, \ldots, 9, A, B, C, D, E, F,$ — hexadecimal

Base-10:

For example: $3773 = 3 \times 10^3 + 7 \times 10^2 + 7 \times 10 + 3$.

Right-most digit: represents a number from 0 to 9;
second from right: represents a multiple of 10;
$\ldots$.

$$3 \quad 7 \quad 7 \quad 3 \quad = \quad 3 \quad + \quad 7\text{x}10 \quad + \quad 7\text{x}10^2 \quad + \quad 3\text{x}10^3$$

Figure 1: Positional notation of a base-10 number

Positional notation: different position represents different magnitude.

Base-2: sequence of 0 and 1

Primary logic units of digital computers are ON/OFF components.

Bit: each binary digit is referred to as a bit.

For example: $(1011)_2 = 1 \times 2^3 + 1 \times 2^1 + 1 = (11)_{10}$

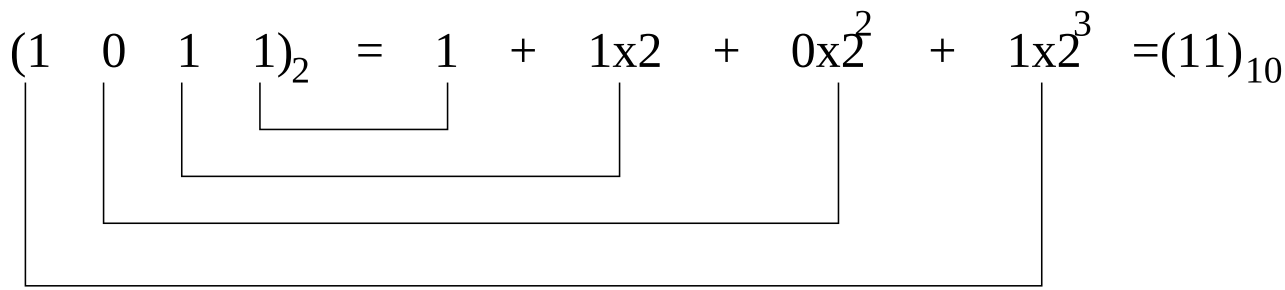


Figure 2: Positional notation of a base-2 number

1.2 Binary representation of integers

Signed magnitude method

The sign bit is used to represent positive as well as negative numbers:

$$\text{sign bit} = 0 \quad \rightarrow \quad \text{positive number}$$
$$\text{sign bit} = 1 \quad \rightarrow \quad \text{negative number}$$

Examples: 8-bit representation

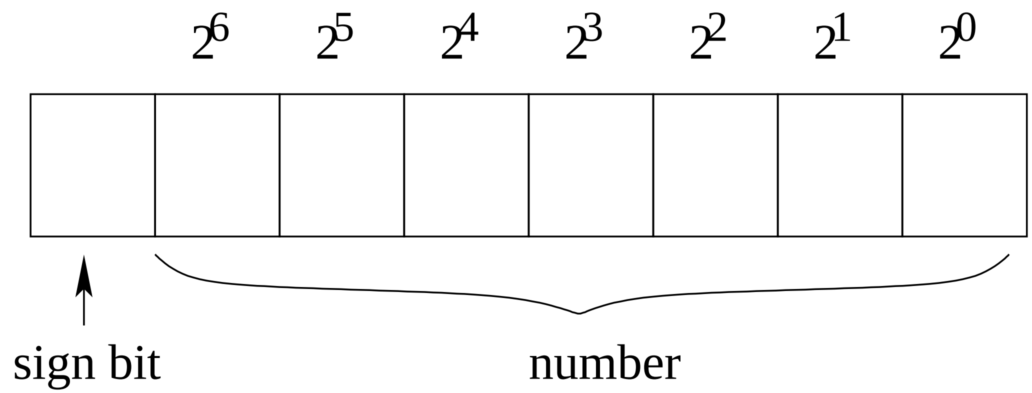


Figure 3: 8-bit representation of an integer with a sign bit

$$(00011000)_2 = (2^4 + 2^3) = (24)_{10}$$
$$(10011000)_2 = -(2^4 + 2^3) = (-24)_{10}$$

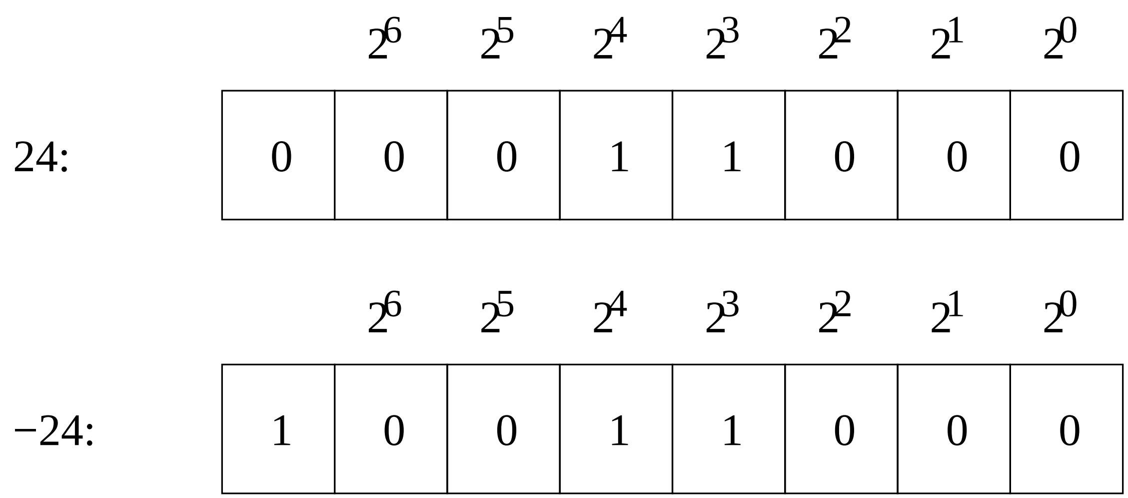


Figure 4: Signed magnitude representation of $(24)_{10}$ and -24_{10}

Maximum number in 8-bit representation: $(01111111)_2 = \sum_{i=0}^{6} 1 \times 2^i = 127.$

Minimum number in 8-bit representation: $(11111111)_2 = -\sum_{i=0}^{6} 1 \times 2^i = -127.$

The range of representable numbers in 8-bit signed representation is from -127 to 127.

In general, with n bits (including one sign bit), the range of representable numbers is $-(2^{n-1} - 1)$ to $2^{n-1} - 1$.

2's complement representation

A computer stores 2's complement of a number.

How to find 2's complement of a number:

i) The 2's complement of a positive integer is the same:
$(24)_{10} = (00011000)_2$

ii) The 2's complement of a negative integer: Negative 2's complement numbers are represented as the binary number that when added to a positive number of the same magnitude equals zero.

- toggle the bits of the positive integer: $(00011000)_2 \quad \rightarrow \quad (11100111)_2$
- add 1 $\quad (11100111 + 1)_2 = (11101000)_2$

$$(24)_{10} = (0\ 0\ 0\ 1\ 1\ 0\ 0\ 0)_2$$

$$
\begin{array}{lrcccccccc}
\text{Toggle bits:} & & 1 & 1 & 1 & 0 & 0 & 1 & 1 & 1 \\
\text{Add 1:} & +) & & & & & & & & 1 \\
\hline
& & 1 & 1 & 1 & 0 & 1 & 0 & 0 & 0
\end{array}
$$

Figure 5: 2's complement representation of -24

$$(128)_{10} = (1\ 0\ 0\ 0\ 0\ 0\ 0\ 0)_2$$

$$
\begin{array}{lrcccccccc}
\text{Toggle bits:} & & 0 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\text{Add 1:} & +) & & & & & & & & 1 \\
\hline
& & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0
\end{array}
$$

Figure 6: 2's complement representation of -128

With 8-bits, representable range: from -128 to 127.

In 2's complement representation, $(10000000)_2 = -128$. The representation 10000000 is not used in signed notation.

With 8 bits, the signed magnitude method can represent all numbers from -127 to 127, while the 2's complement method can represent all numbers from -128 to 127.

2's complement is preferred because of the way arithmetic operations are performed in the computer[1]. In addition, the range of representable numbers is -128 to 127.

1.3 Binary representation of floating point numbers

Consider a decimal floating point number:

$$(37.71)_{10} = 3 \times 10^1 + 7 \times 10^0 + 7 \times 10^{-1} + 1 \times 10^{-2}$$

n-th digit right to "." represents $0 \sim 9 \times 10^{-n}$

Similarly, a binary floating point number:

$$(10.11)_2 = 1 \times 2^1 + 0 \times 2^0 + 1 \times 2^{-1} + 1 \times 2^{-2}$$

n-th digit right to "." represents $0 \sim 1 \times 2^{-n}$

[1] Interested student can visit http://en.wikipedia.org/wiki/Two's_complement for further explanation.

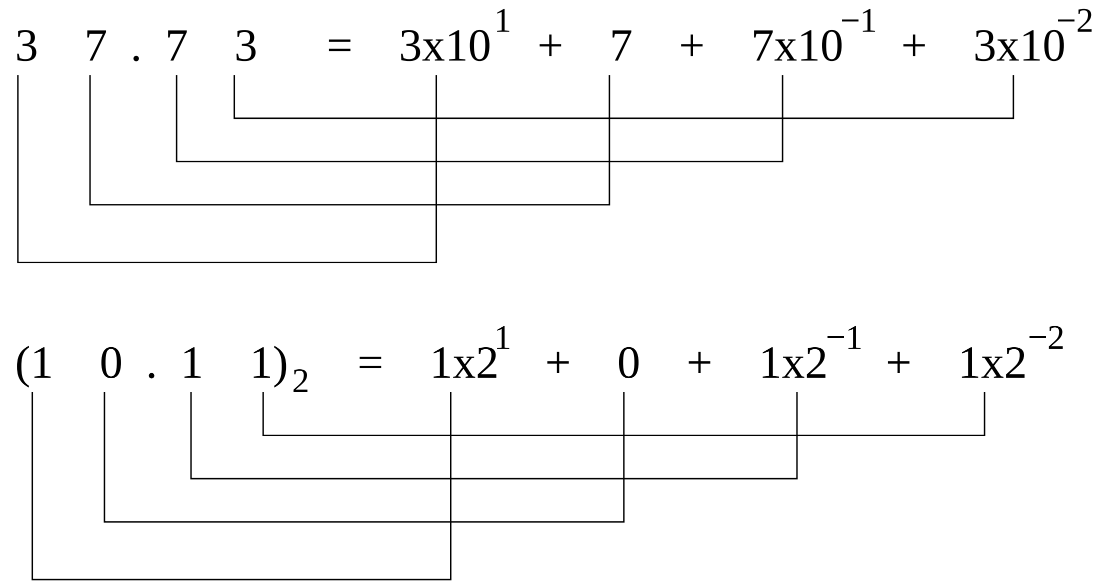


Figure 7: Positional notations of floating point numbers

Normalized representation:

Decimal:

$$37.71 = 3.771 \times 10^1$$
$$0.3771 = 3.771 \times 10^{-1}$$

Idea: move the decimal point to the left or right until there is only one non-zero digit to the left of the point (.) and then compensate for it in the exponent.

Binary:

$$(10.11)_2 = (1.011)_2 \times 2^1$$

$(\times 2^1)$ $\leftrightarrow$ move decimal point one position right
$(\times 2^{-1})$ $\leftrightarrow$ move decimal point one position left

In general, a real number x can be written as

$$x = (-1)^s \cdot m \cdot b^e$$

where
s is the sign bit ($s = 0$ represents positive numbers, and $s = 1$ negative numbers),
m is the mantissa (the normalized value) ($m = 1.f$ for $x \neq 0$ binary),
b is the base ($b = 2$ for binary),
and e is the exponent.

In computers, we store s, m and e. An example of 8-bit representation of floating point numbers is shown in Fig. 8.

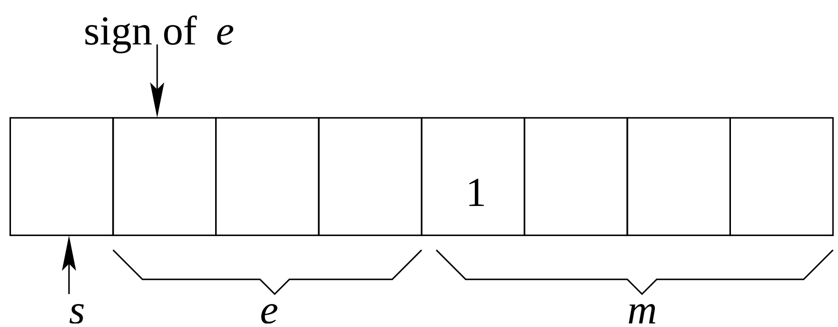


Figure 8: 8-bit floating point normalized representation

Example: $(2.75)_{10} = (10.11)_2 = (1.011)_2 \times 2^1$
The MSB bit of m is always 1, except when $x = 0$. (Why?) Therefore, m can be

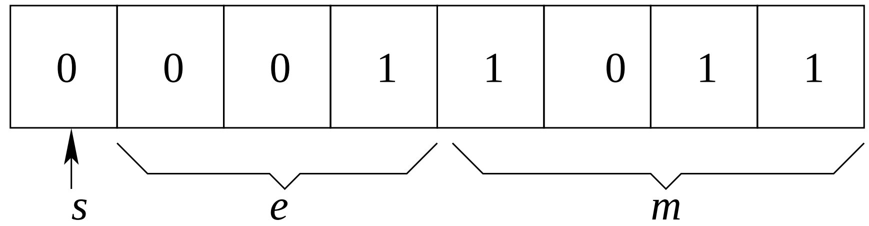


Figure 9: 8-bit floating point normalized representation of 2.75

rewritten as

$$m = (1.f)_2$$

Since only the last three bits carry information, we may exclude the MSB of m and use the last four bits to represent f. Then

$$x = (-1)^s \cdot m \cdot b^e = (-1)^s \cdot (1.f)_2 \cdot b^e$$

For example, $(2.75)_{10} = (1.011)_2 \times 2^1$ can be represented in floating point format as Fig. 10.

In the improved floating point representation, we store s, f and e in computers.

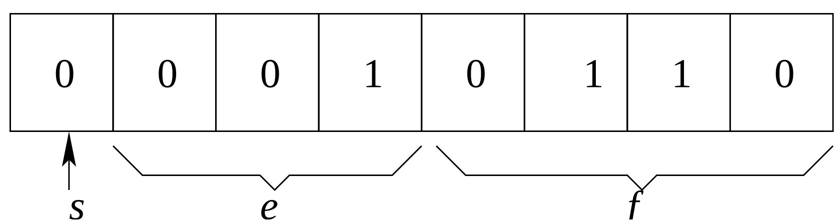


Figure 10: Improved 8-bit floating point normalized representation of 2.75

Special case, $x = 0$.

IEEE standard for floating point representation[2]

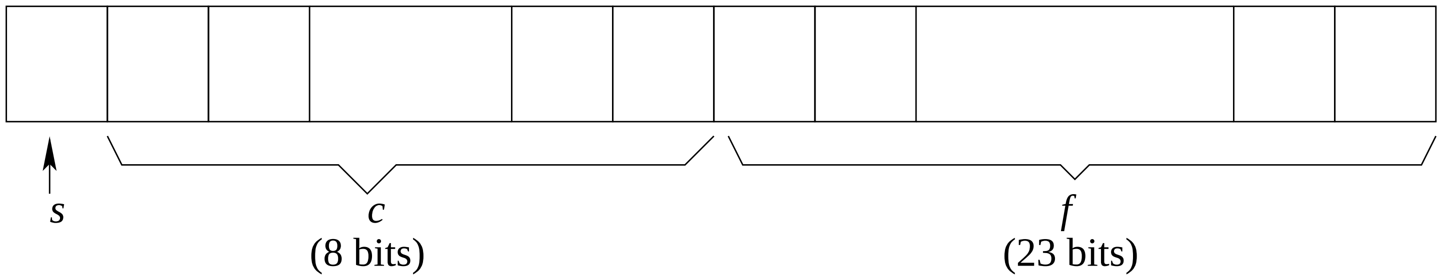


Figure 11: IEEE 32-bit floating point format

In IEEE 32-bit floating point format,

- s(1 bit): sign bit;
- c(8 bits): exponent e with offset, $e = c - 127$, and $c = e + 127$;
  The exponent is not stored directly. The reason for the offset is to make the aligning of the radix point easier during arithmetic operation.
  The range of c is from 0 to 255.
  Special case: $c = 0$ when $x = 0$, and $c = 255$ when x is infinity or not a number (Inf/Nan).
  The valid range of e is from -126 to 127 ($x \neq 0$, Inf, and Nan).
- f(23 bits): $m = (1.f)_2$, ($x \neq 0$, Inf, and Nan), $0 \leq f < 1$.

Example: $2.75 = (10.11)_2 = (1.011)_2 \times 2^1$, where $s = 0$, $m = (1.011)_2$, $e = 1$, and $c = e + 127 = 128 = (10000000)_2$.

[2] More details about the IEEE Standard can be found from http://steve.hollasch.net/cgindex/coding/ieeefloat.html and http://grouper.ieee.org/groups/754/.

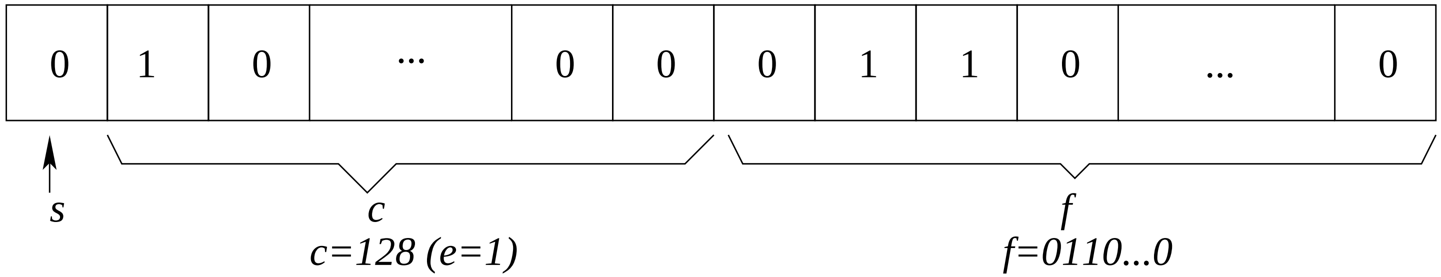


Figure 12: IEEE 32-bit floating point representation of 2.75

1.4 Floating point errors

Using a finite number of bits, for example, as in the IEEE format, only a finite number of real values can be represented exactly. That is, only certain numbers between a minimum and a maximum can be represented.

With the IEEE 32-bit format

- The upper bound U on the representable value of x:
  When $s = 0$, and both c and f are at their maximum values, i.e., $c = 254$ (or $e = 127$), and $f = (11\ldots1)_2$ (or $m = (1.11\ldots1)_2$),
  $$U = m \cdot b^e = (2 - 2^{-23}) \times 2^{127} \approx 3.4028 \times 10^{38}$$
- The lower bound L on the positive representable value of x:
  When $s = 0$, and both c ($c \neq 0$) and f are at their minimum values, i.e., $c = 1$ ($e = c - 127 = -126$), and $f = (00\ldots0)_2$ (when $m = (1.00\ldots0)_2$). Then
  $$L = m \cdot b^e = 1 \times 2^{-126} = 1.1755 \times 10^{-38}$$

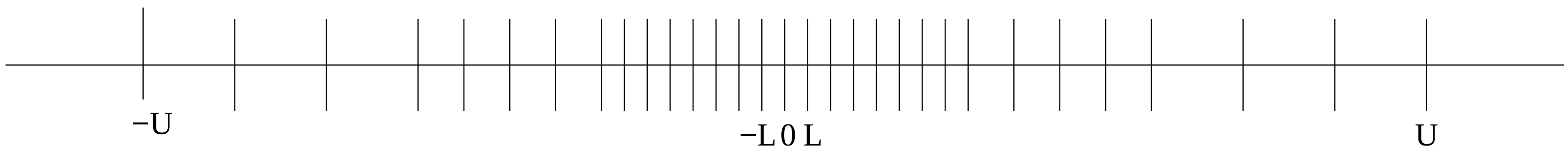


Figure 13: Range of exactly representable numbers

- Only the numbers between $-U$ and $-L$, 0 and between L and U can be represented: $-U \leq x \leq -L$, $x = 0$, or $L \leq x \leq U$.
  During a calculation,
  - when $|x| > U$, the result is in an overflow;
  - when $|x| < L$, the result is in an underflow;
  - if x falls between two exactly representable numbers, its floating point representation has to be approximated, leading to truncation errors.
  - When $|x|$ increases, truncation error increases in general.

2 Truncation errors in floating point representation

When a real value x is stored using its floating point representation $fl(x)$, truncation error occurs. This is because of the need to represent an infinite number of real values using a finite number of bits.

Example: the floating point representation of $(0.1)_{10}$

$$(0.1)_{10} = (0.\ 0001\ 1001\ 1001\ 1001\ 1001\ 1001\ 1001\ \ \ldots)_2$$

2.1 Truncation errors

Assume: we have t number of bits to represent m (or equivalently $t-1$ bits for f). In IEEE 32-bit format, $t-1=23$, or $t=24$.

Figure 14: Truncation error

With a finite number of bits, there are two ways to approximate a number that cannot be represented exactly in floating point format.

Consider real value x which cannot be represented exactly and falls between two floating point representations $fl(x_1)$ and $fl(x_2)$.

Chopping:

$$fl(x) = fl(x_1)$$

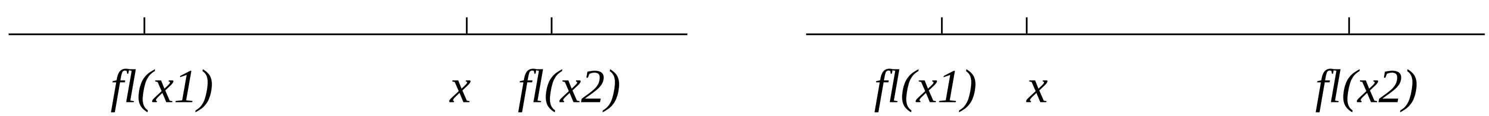
— Ignore all bits beyond the $(t-1)$th one in f (or tth one in m).

Rounding:

$$fl(x) = \begin{cases} fl(x_1), & \text{if } x - fl(x_1) \le fl(x_2) - x \\ fl(x_2), & \text{otherwise.} \end{cases}$$

— Select the closest representable floating point number.

Example: $x > 0$,



Chopping	*fl(x)=fl(x1)*	*fl(x)=fl(x1)*
Rounding	*fl(x)=fl(x2)*	*fl(x)=fl(x1)*

Figure 15: Example of using chopping and rounding

As x increases, $fl(x_2) - fl(x_1)$ increases, then the truncation error increases.

Absolute error:

$$\text{Absolute error} \triangleq |x - fl(x)|$$

is the difference between the actual value and its floating point representation.

Relative error:

$$\text{Relative error} \triangleq \frac{|x - fl(x)|}{|x|}$$

is the error with respect to the value of the number to be represented.

2.2 Bound on the errors ($b = 2$)

Consider chopping, $x > 0$.

The real value x can be represented exactly with an infinite number of bits as

$$x = 1.\underbrace{XX\ldots XX}_{t-1\text{bits}}\underbrace{XX\ldots XX}_{\infty\text{bits}} \times b^e$$

The floating point representation $fl(x)$ is

$$fl(x) = 1.\underbrace{XX\ldots XX}_{t-1\text{bits}} \times b^e$$

The absolute error is maximum when

$$x = 1.\underbrace{XX\ldots XX}_{t-1\text{bits}}\underbrace{11\ldots 11}_{\infty\text{bits}} \times b^e$$

Then, the absolute error is bounded by

$$|x - fl(x)| < \sum_{i=t}^{\infty} b^{-i} \times b^e < b^{-t+1} \times b^e$$

and the relative error is bounded by

$$\frac{|x - fl(x)|}{|x|} < \frac{b^{1-t} \times b^e}{|x|}$$

Because $|x| > 1.00 \cdots 00 \times b^e = b^e$,

$$\frac{|x - fl(x)|}{|x|} < \frac{b^{1-t} \times b^e}{b^e} = b^{1-t}$$

For binary representation, $b = 2$,

$$\frac{|x - fl(x)|}{|x|} < 2^{1-t}$$

which is the bound on relative errors for chopping.

For chopping,

$$|x - fl(x)| \leq [fl(x_2) - fl(x_1)]$$

For rounding: the maximum truncation error occurs when x is in the middle of the interval between $fl(x_1)$ and $fl(x_2)$. Then

$$|x - fl(x)| \leq \frac{1}{2}[fl(x_2) - fl(x_1)]$$

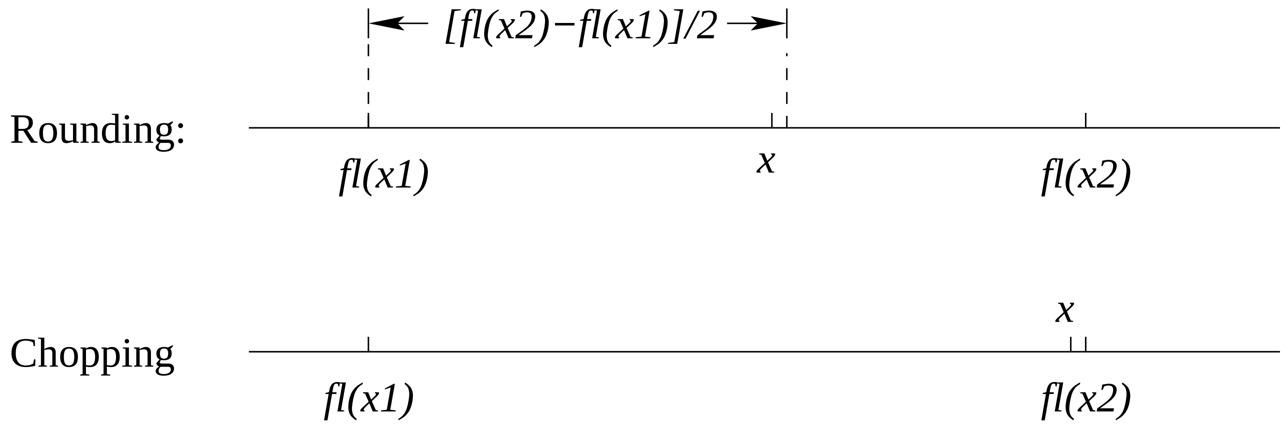


Figure 16: Illustration of error bounds

The bound on absolute errors for rounding is

$$|x - fl(x)| \leq \frac{2^{-t+1} \cdot 2^e}{2} = 2^{-t} \cdot 2^e$$

The bound on relative errors for rounding is

$$\frac{|x - fl(x)|}{|x|} \leq \frac{2^{-t+1}}{2} = 2^{-t}$$

Machine precision: Define machine precision, ϵ_{mach}, as the maximum relative error. Then

$$\epsilon_{mach} = \begin{cases} 2^{1-t}, & \text{for chopping} \\ \frac{2^{1-t}}{2} = 2^{-t}, & \text{for rounding} \end{cases}$$

For IEEE standard, $t-1=23$ or $t=24$, $\epsilon_{mach}=2^{-24}\approx 10^{-7}$ for rounding.
The machine precision ϵ_{mach} is also defined as the smallest number ϵ such that $fl(1+\epsilon)>1$, i.e., if $\epsilon<\epsilon_{mach}$, then $fl(1+\epsilon)=fl(1)$.

(Prove that the two definitions are equivalent.)

Note: Difference between the machine precision, ϵ_{mach}, and the lower bound on the representable floating point numbers, L:

- ϵ_{mach} is determined by the number of bits in m
- L is determined by the number of bits in the exponent e.

2.3 Effects of truncation and machine precision

Example 1: Evaluate $y=(1+\delta)-(1-\delta)$, where $L<\delta<\epsilon_{mach}$. With rounding,

$$\begin{aligned} y &= fl(1+\delta)-fl(1-\delta) \\ &= 1-1=0. \end{aligned}$$

The correct answer should be 2δ.

When $\delta = 1.0 \times 2^{-25}$,

$$\begin{aligned} 1 + \delta &= 1.0 \times 2^0 + 1.0 \times 2^{-25} \\ &= (1.\underbrace{00 \cdots 0}_{24\ 0's}1)_2 \times 2^0 \end{aligned}$$

$$fl(1 + \delta) = 1$$

Example 2: Consider the infinite summation $y = \sum_{n=1}^{\infty} \frac{1}{n}$. In theory, the sum diverges as $n \to \infty$. But, using floating point operations (with finite number of bits), we get a finite output.

As n increases, the addition due to another $\frac{1}{n}$ does not change the output! That is,

$$y = \sum_{n=1}^{\infty} \frac{1}{n} = \sum_{n=1}^{k-1} \frac{1}{n} + \sum_{n=k}^{\infty} \frac{1}{n} = \sum_{n=1}^{k-1} \frac{1}{n}$$

$$\frac{1}{k-1} \geq \epsilon_{mach} \text{ and } \frac{1}{k} < \epsilon_{mach}$$

Example 3: Consider the evaluation of e^{-x}, $x > 0$, using

$$e^{-x} = \sum_{n=0}^{\infty} \frac{(-x)^n}{n!} = 1 - x + \frac{x^2}{2!} - \frac{x^3}{3!} + \dots$$

This may result in erroneous output due to cancellation. Alternative expressions are needed for evaluation with negative exponents.

2.4 Significant figures (digits)

Figure 17: Significant figures

The significant digits of a number are those that can be used with confidence. For example:

$$0.00453 = 4.53 \times 10^{-3} \text{ 3 significant digits}$$

$$0.004530 = 4.530 \times 10^{-3} \text{ 4 significant digits}$$

Example: $\pi = 3.1415926 \cdots$
With 2 significant digits, $\pi \approx 3.1$
With 3 significant digits, $\pi \approx 3.14$
With 4 significant digits, $\pi \approx 3.142$

The number of significant digits is the number of certain digits plus one estimated digit.

3 Approximating a function using a polynomial

3.1 McLaurin series

Assume that $f(x)$ is a continuous function of x, then

$$f(x) = \sum_{i=0}^{\infty} a_i x^i = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} x^i$$

is known as the McLaurin Series, where a_i's are the coefficients in the polynomial expansion given by

$$a_i = \frac{f^{(i)}(x)}{i!}\Big|_{x=0}$$

and $f^{(i)}(x)$ is the i-th derivative of $f(x)$.

The McLaurin series is used to predict the value $f(x_1)$ (for any $x = x_1$) using the function's value $f(0)$ at the "reference point" ($x = 0$). The series is approximated by summing up to a suitably high value of i, which can lead to approximation or truncation errors.

Problem: When function $f(x)$ varies significantly over the interval from $x = 0$ to $x = x_1$, the approximation may not work well.

A better solution is to move the reference point closer to x_1, at which the function's polynomial expansion is needed. Then, $f(x_1)$ can be represented in terms of $f(x_r)$, $f^{(1)}(x_r)$, etc.

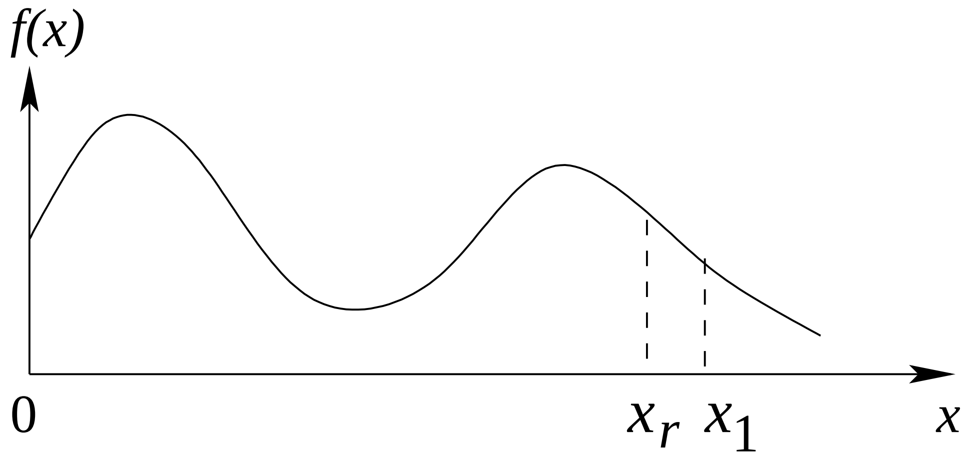


Figure 18: Taylor series

3.2 Taylor series

Assume that $f(x)$ is a continuous function of x, then

$$f(x) = \sum_{i=0}^{\infty} a_i (x - x_r)^i$$

where $a_i = \frac{f^{(i)}(x)}{i!}|_{x=x_r}$. Define $h = x - x_r$. Then,

$$f(x) = \sum_{i=0}^{\infty} a_i h^i = \sum_{i=0}^{\infty} \frac{f^{(i)}(x_r)}{i!} h^i$$

which is known as the Taylor Series.

If x_r is sufficiently close to x, we can approximate $f(x)$ with a small number of coefficients since $(x - x_r)^i \to 0$ as i increases.

Question: What is the error when approximating function $f(x)$ at x by $f(x) = \sum_{i=0}^{n} a_i h^i$, where n is a finite number (the order of the Taylor series)?

Taylor theorem:

A function $f(x)$ can be represented exactly as

$$f(x) = \sum_{i=0}^{n} \frac{f^{(i)}(x_r)}{i!} h^i + R_n$$

where R_n is the remainder (error) term, and can be calculated as

$$R_n = \frac{f^{(n+1)}(\alpha)}{(n+1)!} h^{n+1}$$

and α is an unknown value between x_r and x.

- Although α is unknown, Taylor's theorem tells us that the error R_n is proportional to h^{n+1}, which is denoted by

  $$R_n = O(h^{n+1})$$

  which reads "R_n is order h to the power of $n+1$".

- With n-th order Taylor series approximation, the error is proportional to step size h to the power $n+1$. Or equivalently, the truncation error goes to zero no slower than h^{n+1} does.

- With $h \ll 1$, an algorithm or numerical method with $O(h^2)$ is better than one with $O(h)$. If you half the step size h, the error is quartered in the former but is only halved in the latter.

Question: How to find R_n?

$$\begin{aligned} R_n &= \sum_{i=0}^{\infty} a_i h^i - \sum_{i=0}^{n} a_i h^i \\ &= \sum_{i=n+1}^{\infty} a_i h^i = \sum_{i=n+1}^{\infty} \frac{f^{(i)}(x_r)}{i!} h^i \end{aligned}$$

For small h ($h \ll 1$),

$$R_n \approx \frac{f^{(n+1)}(x_r)}{(n+1)!} h^{n+1}$$

The above expression can be used to evaluate the dominant error terms in the n-th order approximation.

For different values of n (the order of the Taylor series), a different trajectory is fitted (or approximated) to the function. For example:

- $n = 0$ (zero order approximation) $\rightarrow$ straight line with zero slope
- $n = 1$ (first order approximation) $\rightarrow$ straight line with some slope
- $n = 2$ (second order approximation) $\rightarrow$ quadratic function

Example 1: Expand $f(x) = e^x$ as a McLaurin series.

Solution:

$$a_0 = f(0) = e^0 = 1,$$
$$a_1 = \frac{f'(x)}{1!}|_{x=0} = \frac{e^0}{1} = 1$$
$$a_i = \frac{f^{(i)}(x)}{i!}|_{x=0} = \frac{e^0}{i!} = \frac{1}{i!}$$

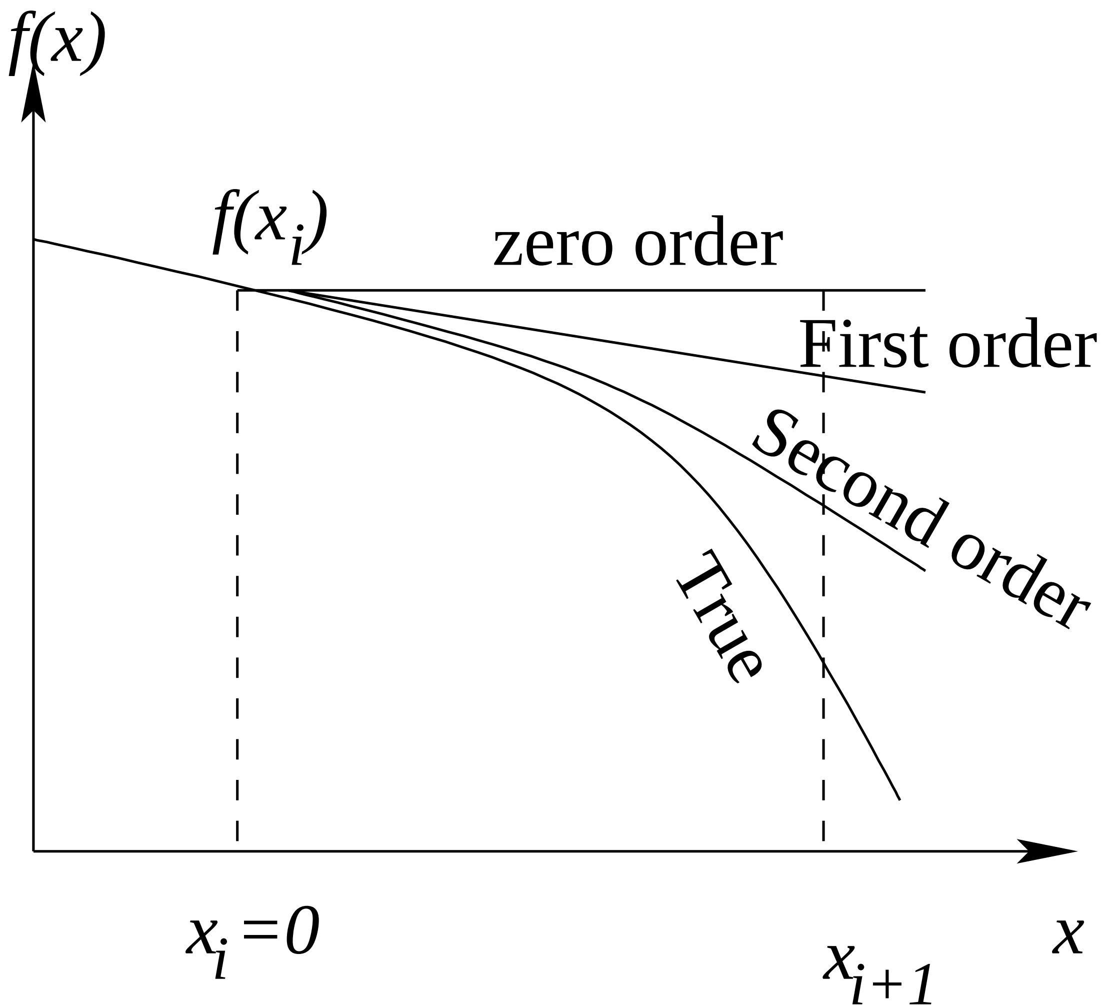


Figure 19: Taylor series

Then $f(x) = e^x = \sum_{i=0}^{\infty} \frac{x^i}{i!}$.

Example 2: Find the McLaurin series up to order 4, Taylor series (around $x = 1$) up to order 4 of function $f(x) = x^3 - 2x^2 + 0.25x + 0.75$.

Solution:

$$
\begin{array}{lll}
f(x) = x^3 - 2x^2 + 0.25x + 0.75 & f(0) = 0.75 & f(1) = 0 \\
f^{'}(x) = 3x^2 - 4x + 0.25 & f^{'}(0) = 0.25 & f^{'}(1) = -0.75 \\
f^{''}(x) = 6x - 4 & f^{''}(0) = -4 & f^{''}(1) = 2 \\
f^{(3)}(x) = 6 & f^{(3)}(0) = 6 & f^{(3)}(1) = 6 \\
f^{(4)}(x) = 0 & f^{(4)}(0) = 0 & f^{(4)}(1) = 0
\end{array}
$$

The McLaurin series of $f(x) = x^3 - 2x^2 + 0.25x + 0.75$ can be written as

$$
f(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(0)}{i!} x^i = \sum_{i=0}^{3} \frac{f^{(i)}(0)}{i!} x^i
$$

Then the third order McLaurin series expansion is

$$
\begin{aligned}
f_{M3}(x) &= f(0) + f^{'}(0)x + \frac{1}{2} f^{''}(0)x^2 + \frac{1}{3!} f^{(3)}(0)x^3 \\
&= 0.75 + 0.25x - 2x^2 + x^3
\end{aligned}
$$

which is the same as the original polynomial function.

The lower order McLaurin series expansion may be written as

$$\begin{aligned} f_{M2}(x) &= f(0) + \frac{1}{2}f^{''}(0)x^2 \\ &= 0.75 + 0.25x - 2x^2 \\ f_{M1}(x) &= 0.75 + 0.25x \\ f_{M0}(x) &= 0.75 \end{aligned}$$

The Taylor series can be written as

$$f(x) = \sum_{i=0}^{\infty} \frac{f^{(i)}(x_r)}{i!}(x - x_r)^i = \sum_{i=0}^{3} \frac{f^{(i)}(1)}{i!}(x-1)^i$$

Then the third order Taylor series of $f(x)$ is

$$\begin{aligned} f_{T3}(x) &= f(1) + f^{'}(1)(x-1) + \frac{1}{2}f^{''}(1)(x-1)^2 + \frac{1}{3!}f^{(3)}(1)(x-1)^3 \\ &= 0.75 + 0.25x - 2x^2 + x^3 \end{aligned}$$

which is the same as the original function.

The lower order Taylor series expansion may be written as

$$\begin{aligned}
f_{T2}(x) &= f(1) + \frac{1}{2}f^{''}(1)(x-1)^2 \\
&= -0.75(x-1) + (x-1)^2 \\
&= 1.75 - 2.75x + x^2 \\
f_{T1}(x) &= f(1) + f^{'}(x-1) \\
&= -0.75(x-1) = 0.75 - 0.75x \\
f_{T0}(x) &= f(1) = 0
\end{aligned}$$

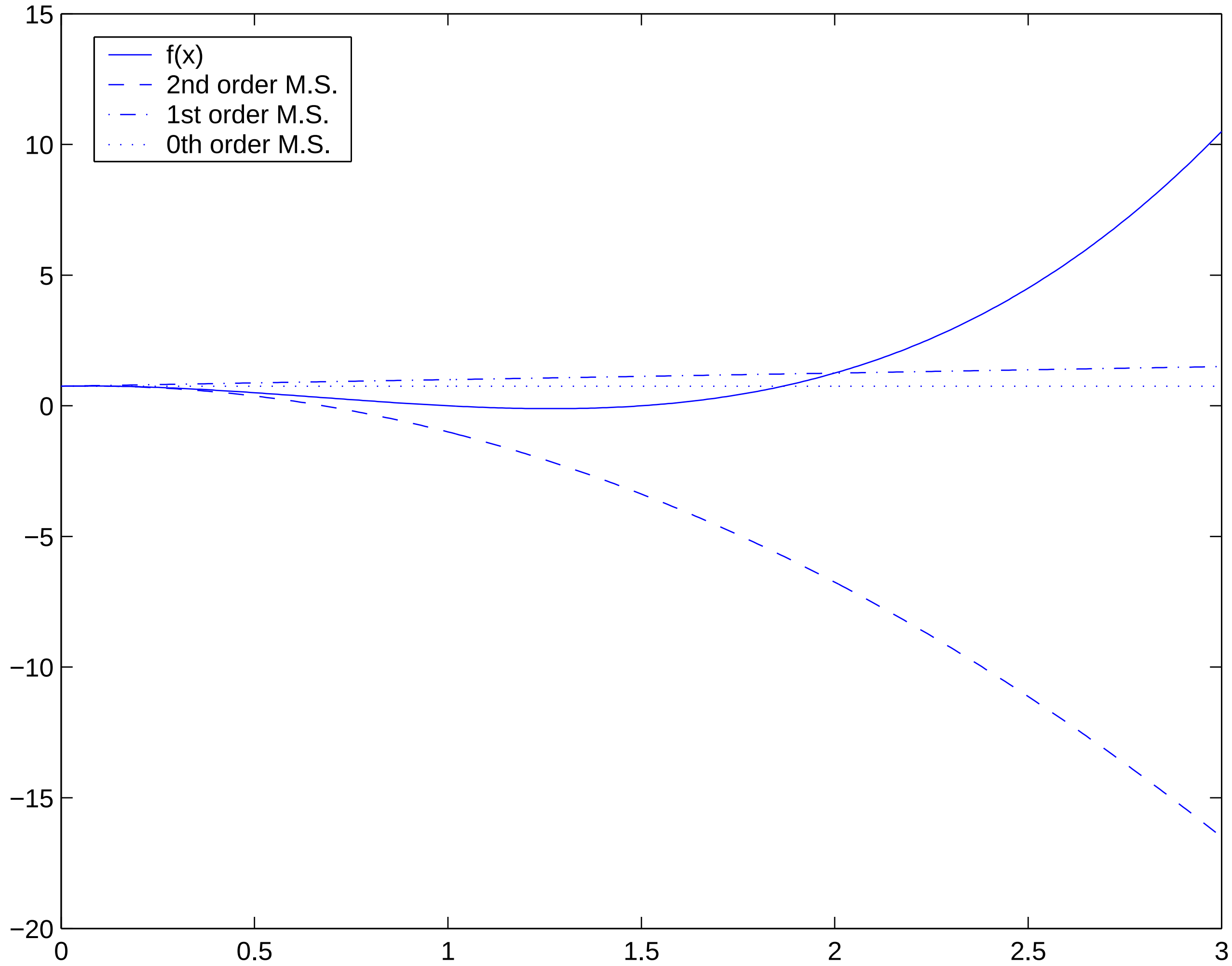


Figure 20: Example 1

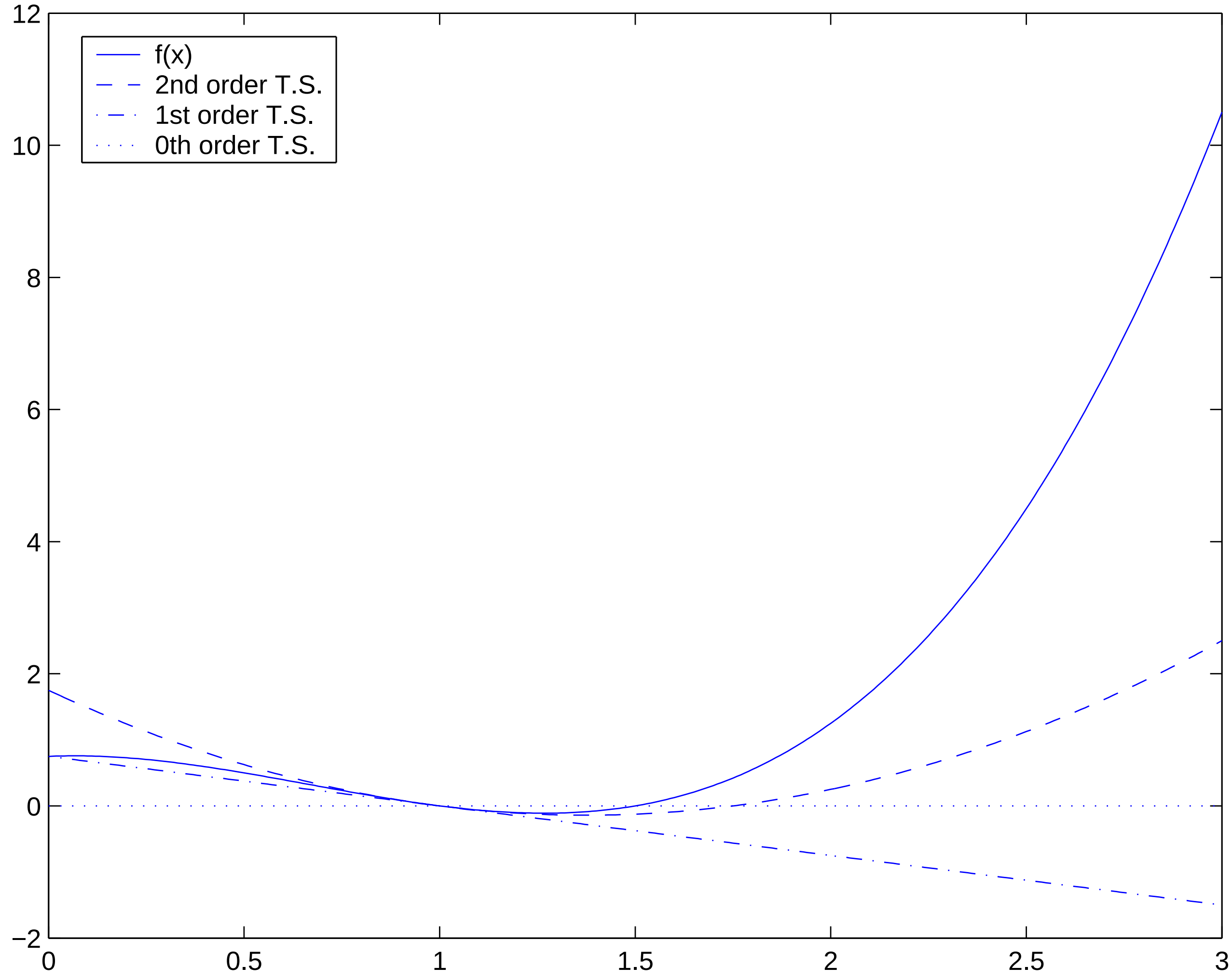


Figure 21: Example 2