Numerical Methods Preliminaries

Professor PhD Henry Arguello Fuentes

Universidad Industrial de Santander
Colombia

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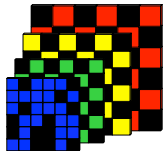
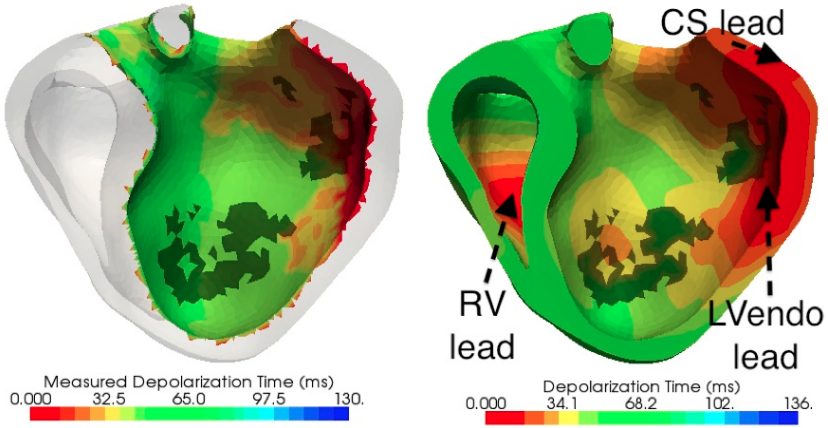


High Dimensional Signal Processing Group
www.hdspgroup.com
henarfu@uis.edu.co
LP 304

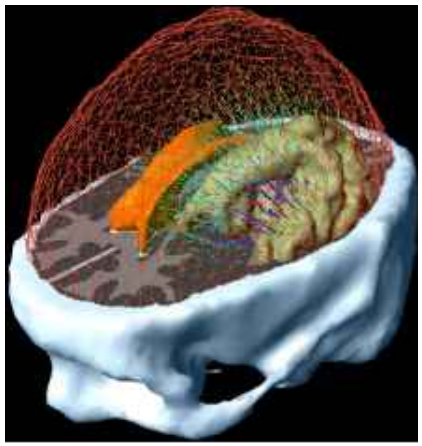
Outline

Introduction: numerical methods applications

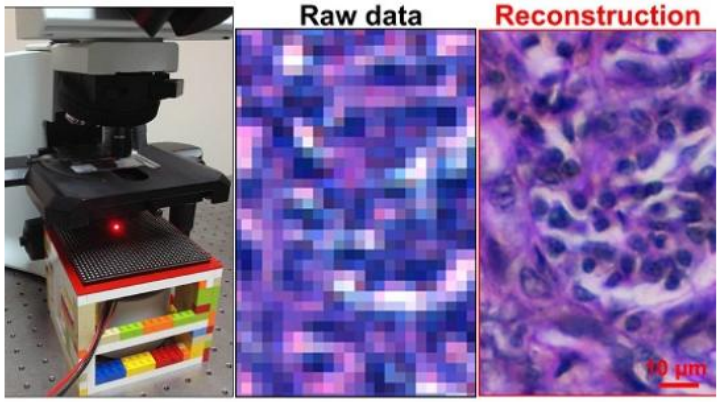
(a) Model the probable evolution of a pathology



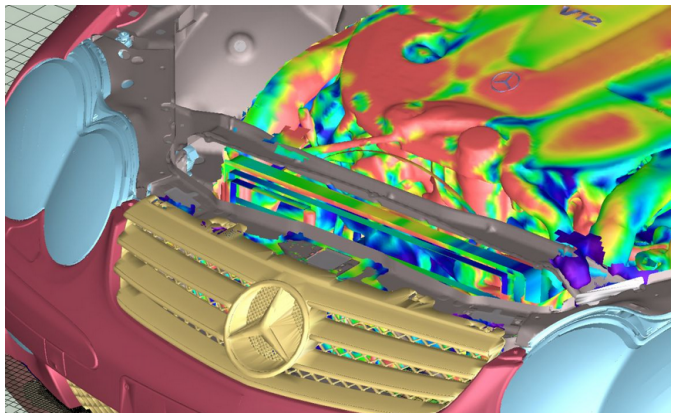
(b) Model and simulate the growth of a tumor



(c) Microscopy super-resolution



(d) Thermal management



Contents

Base 2 numbers

Base 10 numbers: Expanded form of the number 1563

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Let N denote a positive integer; then the digits $a_0, a_1, ..., a_k$ exist so that N has the base 10 expansion

Base 10 expansion

$$N = (a_k \times 10^k) + (a_{k-1} \times 10^{k-1}) + \cdots + (a_1 \times 10^1) + (a_0 \times 10^0), \quad (1)$$

Where the digits a_k are chosen from $0, 1, ..., 8, 9$.

Base 2 numbers

Base 2 numbers: Expanded form of the number 1563

$$\begin{aligned}1563 =&(1\times 2^{10})+(1\times 2^{9})+(0\times 2^{8})+(0\times 2^{7})+(0\times 2^{6})+(0\times 2^{5})+\\&(1\times 2^{4})+(1\times 2^{3})+(0\times 2^{2})+(1\times 2^{1})+(1\times 2^{0}).\end{aligned}$$

So that:

$$1563 = 1024+512+16+8+2+1.$$

Base 2 numbers

Let N denote a positive integer; the digits $b_0, b_1, ..., b_J$ exist so that N has the base 2 expansion

Base 2 expansion

$$N = (b_J \times 2^J) + (b_{J-1} \times 2^{J-1}) + \cdots + (b_1 \times 2^1) + (b_0 \times 2^0), \quad (2)$$

Where each digit b_j is either a 0 or 1. Thus N is expressed in binary notation as

$$N = b_J b_{J-1} \cdots b_2 b_1 b_{0two}. \quad (3)$$

Contents

Base 2 representation of the integer N

Process: Generate sequences Q_k and R_k of quotients and remainders, respectively. End the process when $Q_k = 0$, for some integer $k = J$.

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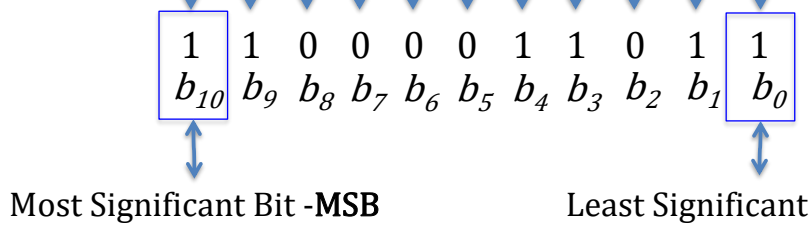
Example:

k	1563	Q_k	R_k
0	1563/2=	781	1
1	781/2=	390	1
2	390/2=	195	0
3	195/2=	97	1
4	97/2=	48	1
5	48/2=	24	0
6	24/2=	12	0
7	12/2=	6	0
8	6/2=	3	0
9	3/2=	1	1
10	1/2=	0	1



Base 2 representation of the integer N

Exercise 1: Find the base 2 representation of 697

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- Start by dividing the integer N from 2 to calculate Q_0 and R_0.

$$697/2 = 348.5 \rightarrow Q_0 = 348 \text{ and } R_0 = 1$$

Base 2 representation of the integer N

Exercise 1: Find the base 2 representation of 697

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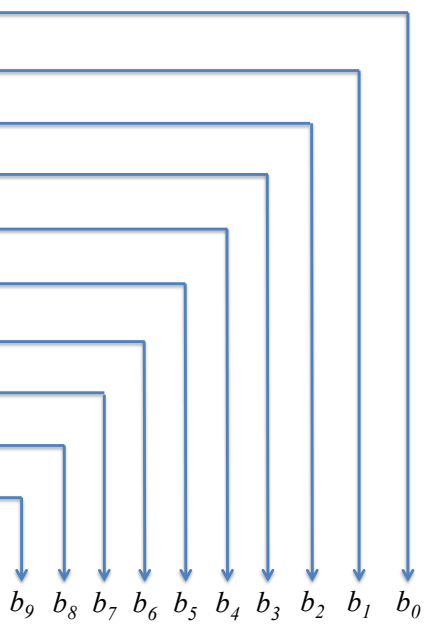
$$697/2 = 348.5 \rightarrow Q_0 = 348 \text{ and } R_0 = 1$$

- Continue the process until finding $Q_k = 0$, for some integer $k = J$.

$$Q_k = Q_{k-1}/2$$

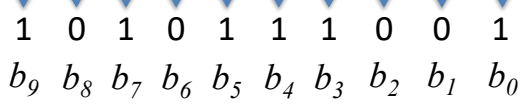
k	697	Q_k	R_k
0	697/2=	348	1
1			
2			
3			
4			
5			
6			
7			
8			
9			



Base 2 representation of the integer N

Solution

k	697	Q_k	R_k
0	$697/2=$	348	1
1	$348/2=$	174	0
2	$174/2=$	87	0
3	$87/2=$	43	1
4	$43/2=$	21	1
5	$21/2=$	10	1
6	$10/2=$	5	0
7	$5/2=$	2	1
8	$2/2=$	1	0
9	$1/2=$	0	1



Then, $697_{10} = 1010111001_2$

Contents

Commonly, when you express a rational number in decimal form, you require infinitely many digits.

For example, in $\frac{1}{3} = 0.\overline{3}$, the symbol $\overline{3}$ means that the digit 3 is repeated forever to form an infinite repeating decimal.

But, the number $\frac{1}{3}$ is the shorthand notation for the infinite series S

$$S = (3 \times 10^{-1}) + (3 \times 10^{-2}) + \cdots + (3 \times 10^{-\infty})$$

$$S = \sum_{k=1}^{\infty} 3(10)^{-k} = \frac{1}{3}.$$

Definition 1.

The infinite series S

$$S = \sum_{n=0}^{\infty} cr^n = c + cr + cr^2 + \cdots + cr^n + \cdots , \tag{4}$$

where $c \neq 0$ and $r \neq 0$, is called a *geometric series* with ratio r.

Definition 1.

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$$S = \sum_{n=0}^{\infty} cr^n = c + cr + cr^2 + \cdots + cr^n + \cdots , \tag{4}$$

where $c \neq 0$ and $r \neq 0$, is called a *geometric series* with ratio r.

Theorem 1. (Geometric Series)

The geometric series has the following properties:

$$\text{If } |r| < 1, \text{ then } \sum_{n=0}^{\infty} cr^n = \frac{c}{1-r}. \tag{5}$$

$$\text{If } |r| > 1, \text{ then the series diverges.}$$

Example: The series S is given by

$$S = (7)\left(\frac{1}{7}\right)^1 + (7)\left(\frac{1}{7}\right)^2 + \cdots + (7)\left(\frac{1}{7}\right)^{\infty} = \sum_{n=1}^{\infty} 7\left(\frac{1}{7}\right)^n,$$

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$$\text{which is equal to} \quad -7 + \sum_{n=0}^{\infty} 7\left(\frac{1}{7}\right)^n,$$

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$$\text{which is equal to} \quad -7 + \sum_{n=0}^{\infty} 7\left(\frac{1}{7}\right)^n,$$

$$\text{and acording with (5)} \quad S = -7 + \frac{7}{1 - \frac{1}{7}} = \frac{7}{6} = 1.1\overline{6},$$

Then, $\frac{7}{6}$ is the shorthand notation for the infinite series S

Contents

Binary Fractions

A binary fraction is a serie of sums with negative powers of 2, which is used to express a real number R that lies in the range $0 < R < 1$.

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Binary fractions

$$R = (d_1 \times 2^{-1}) + (d_2 \times 2^{-2}) + \cdots + (d_n \times 2^{-n}) + \cdots, \tag{6}$$

where $d_j \in 0, 1$ and $0 < R < 1$.

Binary fraction

$$R = 0.d_1 d_2 \cdots d_n \cdots_{two}$$

Representation of R

$$R = \sum_{j=1}^{\infty} d_j (2)^{-j}$$

Binary Fractions-Decimal to binary

Process: Generate sequences d_k and F_k multiplying by two.

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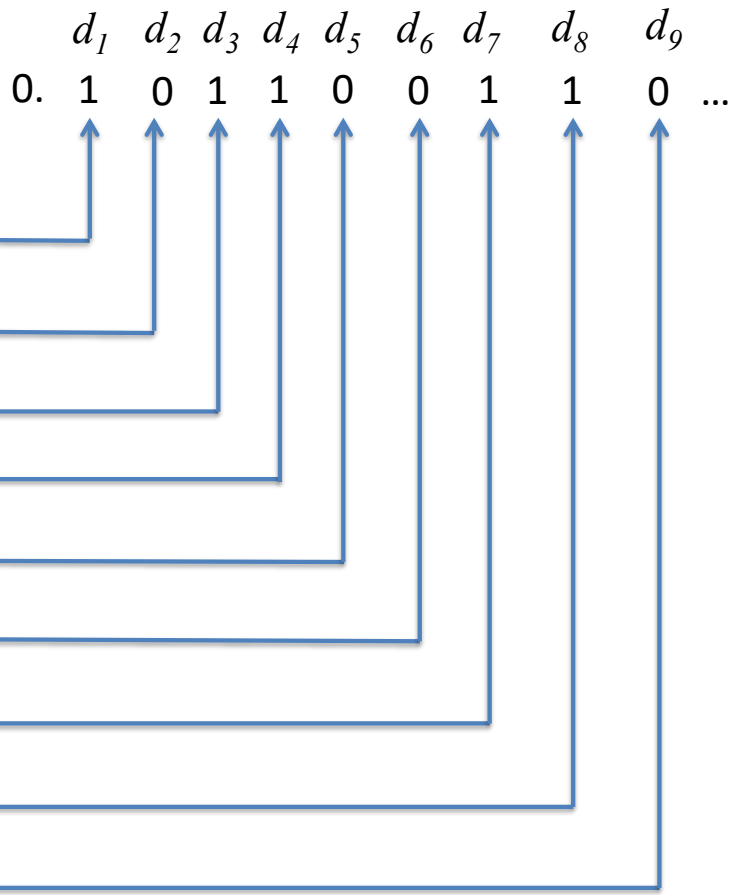
Example:

j	0.7	F_j	d_j	$frac$
1	$(0.7)(2) =$	1.4	1	0.4
2	$(0.4)(2) =$	0.8	0	0.8
3	$(0.8)(2) =$	1.6	1	0.6
4	$(0.6)(2) =$	1.2	1	0.2
5	$(0.2)(2) =$	0.4	0	0.4
6	$(0.4)(2) =$	0.8	0	0.8
7	$(0.8)(2) =$	1.6	1	0.6
8	$(0.6)(2) =$	1.2	1	0.2
9	$(0.2)(2) =$	0.4	0	0.4
⋮	⋮	⋮	⋮	⋮

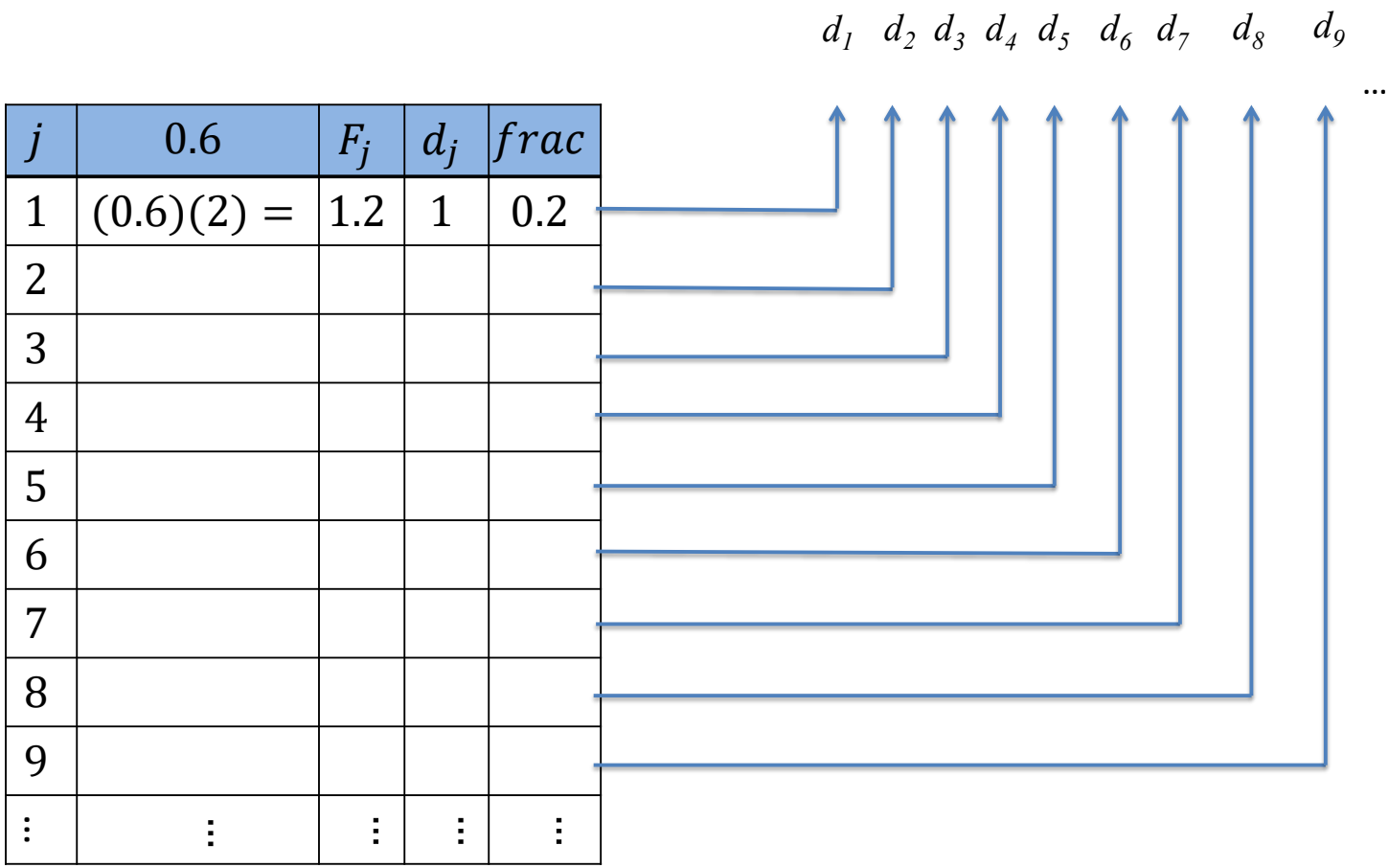


$$0.7 = 0.\overline{10110}_2$$

Binary Fractions-Decimal to binary

Exercise 2: Calculate the binary fraction for 0.6.

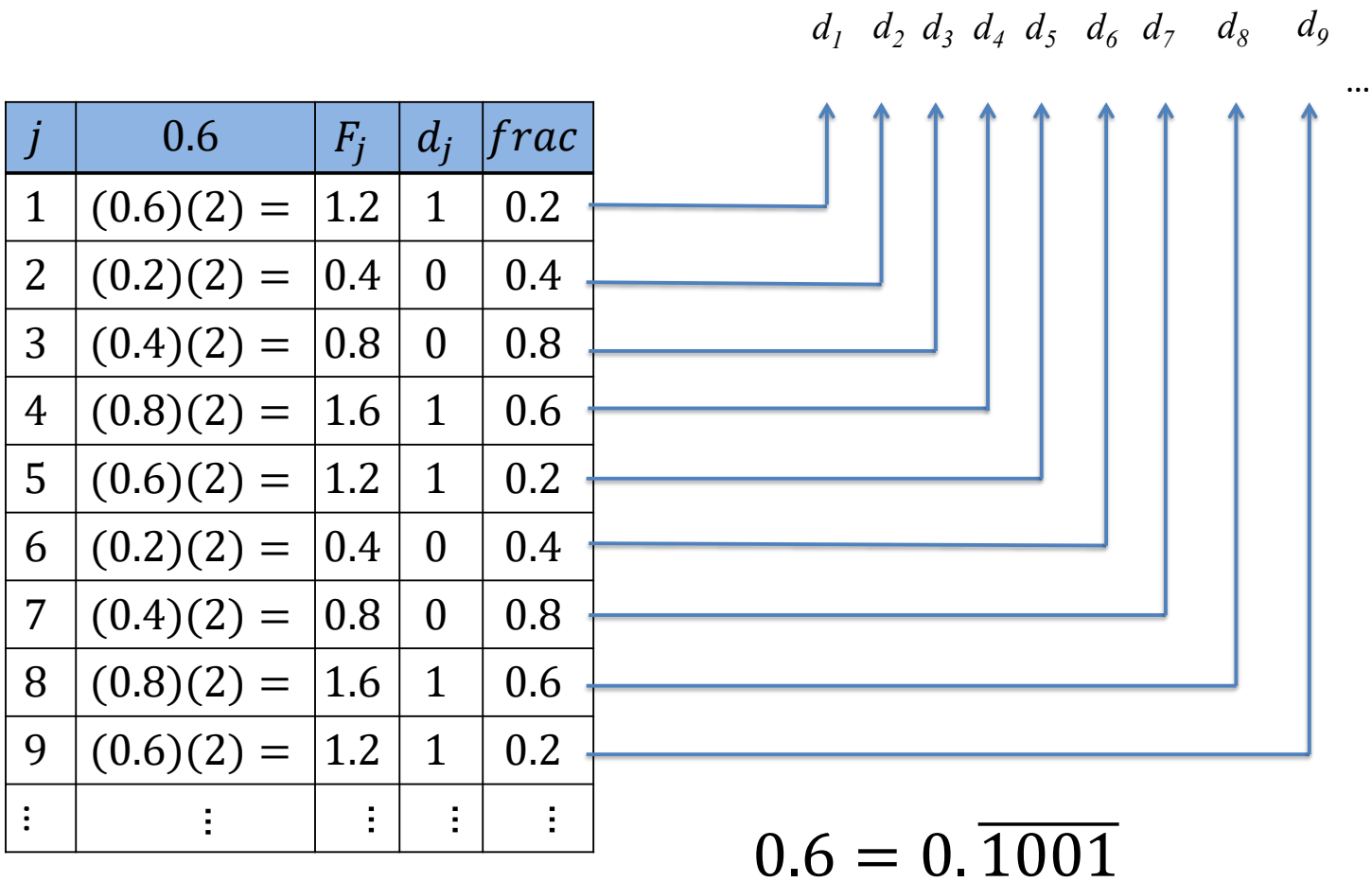
- Start by multiplying 0.6 by 2, to generate sequences d_j and F_j



j	0.6	F_j	d_j	$frac$
1	$(0.6)(2) =$	1.2	1	0.2
2				
3				
4				
5				
6				
7				
8				
9				
⋮	⋮	⋮	⋮	⋮

Binary Fractions-Decimal to binary

Solution



j	0.6	F_j	d_j	$frac$
1	$(0.6)(2) =$	1.2	1	0.2
2	$(0.2)(2) =$	0.4	0	0.4
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8	$(0.8)(2) =$	1.6	1	0.6
9	$(0.6)(2) =$	1.2	1	0.2
⋮	⋮	⋮	⋮	⋮

$$0.6 = 0.\overline{1001}$$

Binary Fractions-Binary to decimal

The base 10 rational number R_{10} associated to a base 2 binary fraction R_2 can be found using geometric series.

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The base 10 rational number R_{10} associated to a base 2 binary fraction R_2 can be found using geometric series.

Example:

$$0.\overline{01}_2 = (0 \times 2^{-1}) + (1 \times 2^{-2}) + (0 \times 2^{-3}) + (1 \times 2^{-4}) \cdots$$

the expression above is writted as

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the expression above is writted as

$$= \sum_{k=1}^{\infty} (2^{-2})^k = -1 + \sum_{k=0}^{\infty} (2^{-2})^k$$

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then, $\frac{1}{3}$ is the 10 rational number associated to $0.\overline{01}_2$

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Binary shifting

Let R be

$$R = 0.00000\overline{11000}_2. \tag{7}$$

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Multiplying both sides of (7) by $2^5 = 32$ will **shift** the binary point **5** places to the right	Multiplying both sides of (7) by $2^{10} = 1024$ will **shift** the binary point **10** places to the right
$32R = 0.\overline{11000}_2.$	$1024R = 11000.\overline{11000}_2.$

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$32R = 0.\overline{11000}_2.$	$1024R = 11000.\overline{11000}_2.$

Taking the difference $1024R - 32R = 11000.\overline{11000}_2 - 0.\overline{11000}_2,$

we obtain $992R = 11000_2,$

given that $11000_2 = 24_{10}$ we find that,

$992R = 24$, Therefore $R = \frac{3}{124}_{10}.$

Contents

Scientific Notation

The scientific notation is a standard way to present a real number. It is obtained by properly shifting the decimal point.

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Examples

- $0.0000747 = 7.47 \times 10^{-5}$
- $31.4159265 = 3.14159265 \times 10$
- $9,700,000.000 = 9.7 \times 10^{9}$
- The Avogadro's constant used in chemistry $= 6.02252 \times 10^{23}$.
- The quantity $1K = 1.024 \times 10^{3}$ used in computer science.

Contents

Machine Numbers

A mathematical quantity x is stored in a computer as a binary approximation given by

$$x \approx \pm q \times 2^n. \tag{8}$$

- The finite binary number q is the **mantissa**, where $1/2 \leq q \leq 1$.
- The integer n is the **exponent**.

Floating-point format

A real number is stored in a computer as a set of binary numbers expressing:

- The sign
- The exponent
- The mantissa

- The sign is always one bit where, $S = 0$ if, $x > 0$ and $S = 1$, if $x < 0$.
- The amount of bits for the exponent and the mantissa depends on the precision of the machine.

Floating-point format-IEEE 754 standard

Precision	Total	Sign	Exponent	Mantissa	Exponent bias
Single	32 bits	1 bit	8 bits	23 bits	127
Double	64 bits	1 bit	11 bits	52 bits	1023

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Then, the exponent is biased by adjusting its value.

The exponent bias is calculated as $bias = 2^{exp-1} - 1$, where exp indicates the amount of bits for the exponent.

Example:
if $exp = 15$ bits, then, $bias = 2^{15-1} - 1 = 16383$

Floating-point format-IEEE 754 standard

Possible cases:

Sign (S)	Exponent (E)	Mantissa (M)	Value
0-1	All 0 < E < All 1	M	$(-1)^S\ (1.M)(2^{E\text{-bias}})$
0	E=all 1	M=0	$+\infty$
1	E=all 1	M=0	$-\infty$
0-1	E=all 1	M≠0	NaN
0-1	E=all 0	M=0	0
0-1	E=all 0	M≠0	$(-1)^S\ (0.M)(2^{1\text{-bias}})$

Floating-point format

Example: Determine the floating point format to stored the number 59.1875_{10} in a computer with 32 bits of precision.

Floating-point format

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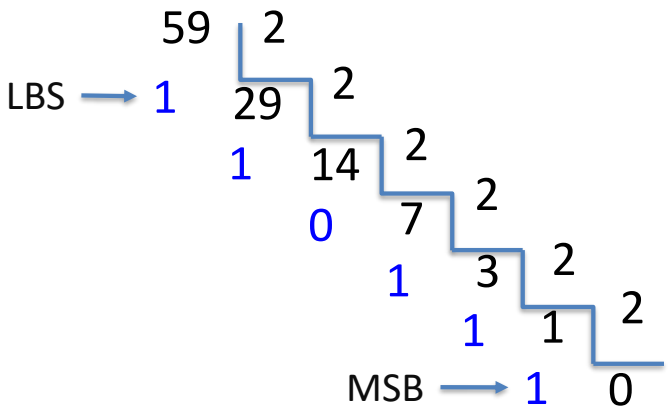
- 1. Find the binary representation of the number 59.1875_{10}

$$59.1875_{10}$$

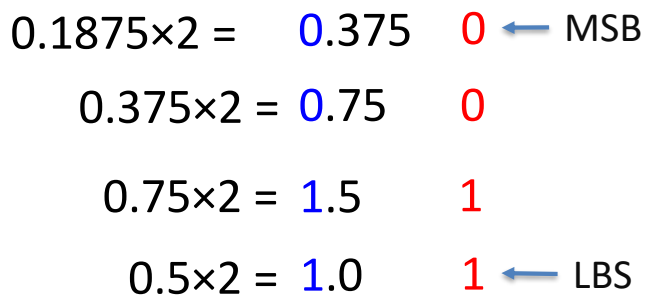
Integer part

$$59_{10}$$



Decimal part

$$0.1875_{10}$$



$$111011.0011_2$$

Floating-point format

- 2. Do the proper binary shifting

$$111011.0011_2 = 1.1101100011_2 \times 2^5$$

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- 3. Calculate the bias

$$bias = 2^{8-1} - 1 = 127$$

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- 4. Determine the mantissa

$$\text{Mantissa} = 110110011_2$$

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- 5. Determine the exponent

$$exp = 5 + bias = 5 + 127 = 132_{10} = 10000100_2$$

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$$111011.0011_2 = 1.110110011_2 \times 2^5$$

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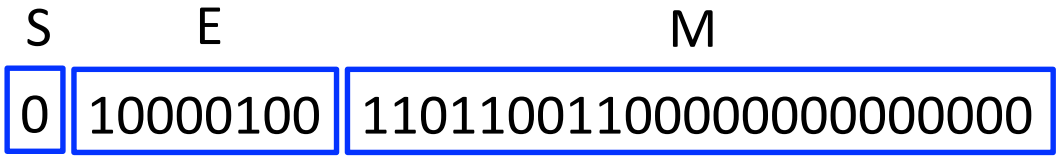
$$exp = 5 + bias = 5 + 127 = 132_{10} = 10000100_2$$



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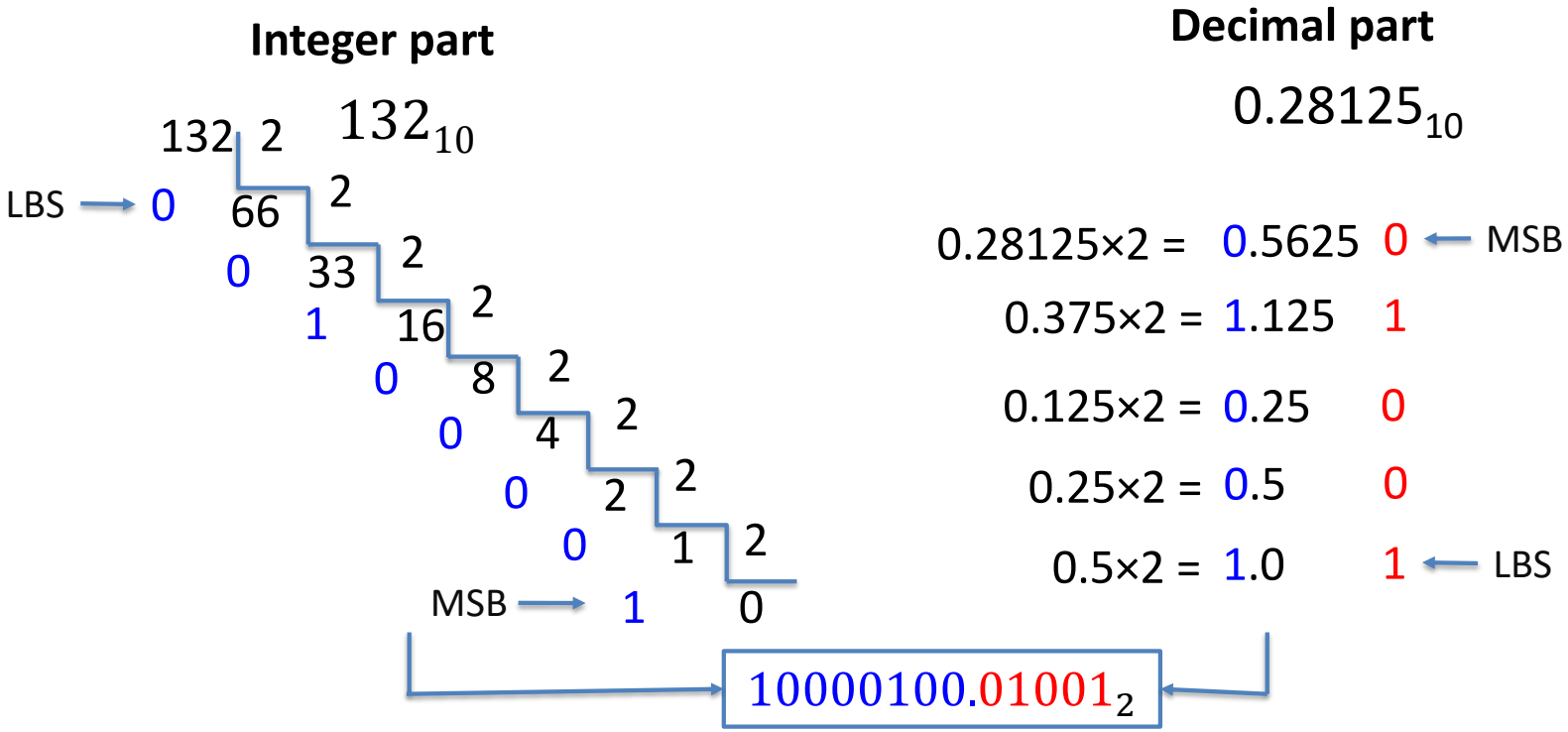
- 1. Find the binary representation of the number 132.28125_{10}

$$132.28125_{10}$$



Floating-point format

- 2. Do the proper binary shifting

$$10000100.01001_2 = 1.0000100001001_2 \times 2^7$$

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$$\text{Mantissa} = 0000100001001_2$$

- 5. Determine the exponent

$$exp = 7 + bias = 7 + 127 = 134_{10} = 10000110_2$$

Floating-point format

- 2. Do the proper binary shifting

$$10000100.01001_2 = 1.0000100010012 \times 2^7$$

- 3. Calculate the bias

$$bias = 2^{8-1} - 1 = 127$$

- 4. Determine the mantissa

$$\text{Mantissa} = 00001000100_2$$

- 5. Determine the exponent

$$exp = 7 + bias = 7 + 127 = 134_{10} = 10000110_2$$

S	E	M
0	10000110	00001000100100000000000

Floating-point format

The real value associated with a given 32 bit binary is calculated as

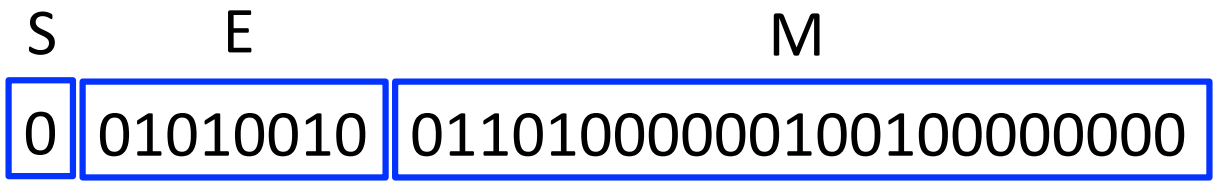
$$value = (-1)^S \left(1 + \sum_{i=1}^{23} d_{(23-i)} 2^{-i}\right) \times 2^{(E-127)}$$

Where,

- S = The sign
- E = Exponent
- 127 = Bias
- d_j = Bits of the mantissa

Floating-point format

Exercise: Find the real value for the binary data:



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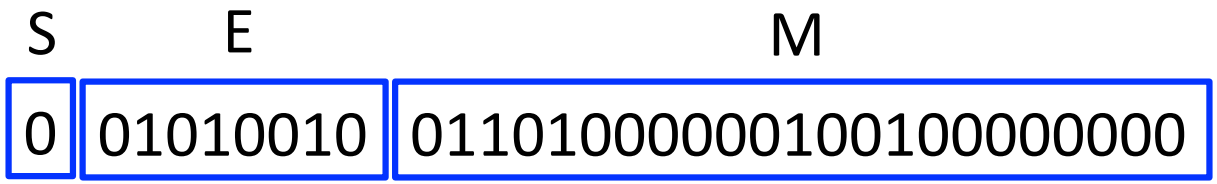

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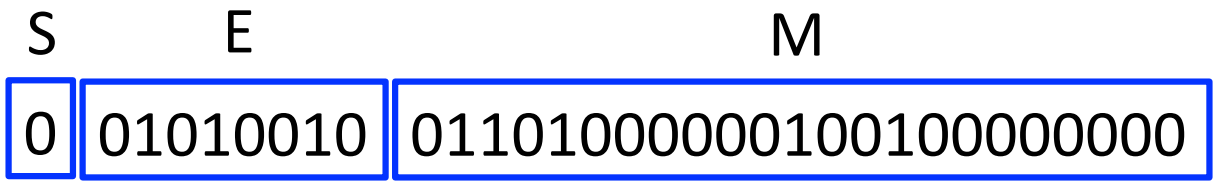

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In this example:

- $S = 0$
- $1 + \sum_{i=1}^{23} d_{(23-i)} 2^{-i} = 1 + 2^{-2} + 2^{-3} + 2^{-5} + 2^{-12} + 2^{-15} = 1.4065246582$
- $2^{(E-127)} = 2^{((2^1+2^4+2^6)-127)} = 2^{82-127} = 2^{-45}$

Floating-point format

Exercise: Find the real value for the binary data:

S	E	M
0	01010010	01101000000100100000000

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Thus

$$value = 1.4065246582 \times 2^{-45}$$

Floating-point format

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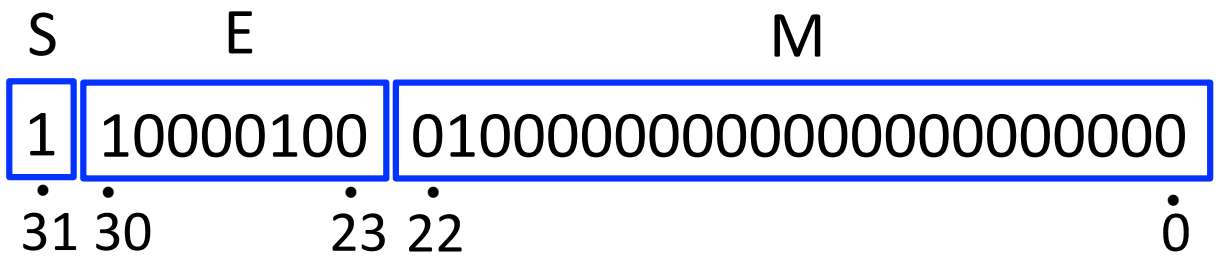
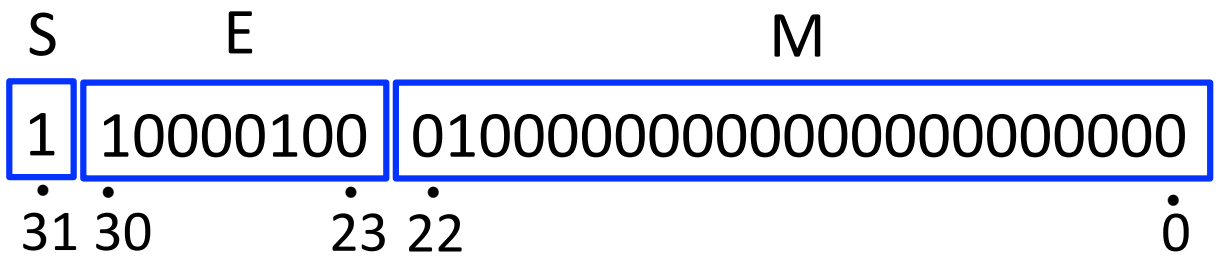


In this example:

- $S = 1$
- $1 + \sum_{i=1}^{23} d_{(23-i)} 2^{-i} = 1 + 2^{-2} = 1.25$
- $2^{(E-127)} = 2^{(132-127)} = 2^5$

Floating-point format

Example: Find the real value for the binary data:



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Thus

$$value = 1.25 \times 2^5 = -40.$$

Contents

Absolute and relative error

Definition 2.

Suppose that $\widehat{p}$ is an approximation to p. The ***absolute error*** is $E_p = |p - \widehat{p}|$, and the ***relative error*** is $R_p = |p - \widehat{p}|/|p|$, provided that $p \neq 0$.

Absolute and relative error

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Suppose that $\widehat{p}$ is an approximation to p. The ***absolute error*** is $E_p = |p - \widehat{p}|$, and the ***relative error*** is $R_p = |p - \widehat{p}|/|p|$, provided that $p \neq 0$.

- The **absolute error** is the difference between the true value and the approximate value.
- The **relative error** expresses the error as a percentage of the true value.

Absolute and relative error

Example: Find the absolute and relative error in the following three cases:

Absolute and relative error

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Real $\lvert p \rvert$	$x = 3.141592$	$y = 1,000,000$	$z = 0.000012$
Approximation $\hat{p}$	$\widehat{x} = 3.14$	$\widehat{y} = 999,996$	$\widehat{z} = 0.000009$
Absolute Error E_p	$E_x = \lvert x - \widehat{x} \rvert$ $= 0.001592$	$E_y = \lvert y - \widehat{y} \rvert$ $= 4$	$E_z = \lvert z - \widehat{z} \rvert$ $= 0.000003$
Relative Error R_p	$R_x = E_x / \lvert x \rvert$ $= 5.067_{\times 10^{-4}}$	$R_y = E_y / \lvert y \rvert$ $= 0.000004$	$R_z = E_z / \lvert z \rvert$ $= 0.25$

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Relative Error R_p	$R_x = E_x/\lvert x\rvert$ $= 5.067_{\times 10^{-4}}$	$R_y = E_y/\lvert y\rvert$ $= 0.000004$	$R_z = E_z/\lvert z\rvert$ $= 0.25$

Observe that as $\lvert p\rvert$ moves away from 1 (greater than or less than) the relative error R_p is a better indicator than E_p of the accuracy of the approximation.

Absolute and relative error

Definition 3.

The number $\widehat{p}$ is said to ***approximate*** p to d significant digits if d is the **largest** nonnegative integer for which

$$\frac{|p-\widehat{p}|}{|p|} < \frac{10^{1-d}}{2}.$$

Absolute and relative error

Example:

Let $\hat{w}$ be the approximation for $w = 2.1645$, then

$$\frac{|2.1645 - 2.16|}{|2.1645|} = 2.07900 \times 10^{-}3$$

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if $d = 2$: $2.07900 \times 10^{-}3 < \frac{10^{1-2}}{2} = 0.05$ ✓satisfies

if $d = 3$: $2.07900 \times 10^{-}3 < \frac{10^{1-3}}{2} = 0.005$ ✓satisfies

if $d = 4$: $2.07900 \times 10^{-}3 < \frac{10^{1-4}}{2} = 0.0005$ X **does not satisfy**

Then, $\hat{w}$ approximate w to 3 significant digits.

Absolute and relative error

Other examples:

- If $x = 3.141592$ and $\widehat{x} = 3.14$, then $|x - \widehat{x}|/|x| = 0.000507 < 10^{-2}/2$. Therefore, $\widehat{x}$ approximates x to three significant digits.
- If $y = 1,000,000$ and $\widehat{y} = 999,996$, then $|y - \widehat{y}|/|y| = 0.000004 < 10^{-5}/2$. Therefore, $\widehat{y}$ approximates y to six significant digits.
- If $z = 0.000012$ and $\widehat{z} = 0.000009$, then $|z - \widehat{z}|/|z| = 0.25 < 10^{-0}/2$. Therefore, $\widehat{z}$ approximates z to one significant digits.

Contents

Truncation Error

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For example, the infinite Taylor series

$$e^{x^2} = 1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \frac{x^8}{4!} + \cdots + \frac{x^{2n}}{n!} + \cdots$$

might be replaced with just the first five terms $1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \frac{x^8}{4!}$. Then a truncation error appears.

Truncation Error

Example: Given $p = \int_0^{1/2} e^{x^2} dx = 0.544987104184$. Determine the accuracy of the approximation obtained by replacing the integrand $f(x) = e^{x^2}$ with the truncated Taylor series $P_8(x) = 1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \frac{x^8}{4!}$.

- Determine $\int_0^{1/2} P_8(x)dx$:

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- Determine $\int_0^{1/2} P_8(x)dx$:

$$\int_0^{1/2} \left(1 + x^2 + \frac{x^4}{2!} + \frac{x^6}{3!} + \frac{x^8}{4!}\right) dx = \left(x + \frac{x^3}{3} + \frac{x^5}{5(2!)} + \frac{x^7}{7(3!)} + \frac{x^9}{9(4!)}\right)\Bigg|_{x=0}^{x=1/2}$$

$$= \frac{1}{2} + \frac{1}{24} + \frac{1}{320} + \frac{1}{5376} + \frac{1}{110592}$$

$$= \frac{2109491}{3870720} = 0.544986720817 = \widehat{p}$$

Since

$$\frac{|p - \widehat{p}|}{|p|} = 7.03442 \times 10^{-7} < \frac{10^{1-6}}{2} = 5 \times 10^{6}$$

then, the approximation $\widehat{p}$ agrees with the true value to 6 significant digits.

Contents

Round-off Error

- The accuracy of the representation of a real number stored in a computer is determined by the precision of the mantissa.

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Round-off Error

- The accuracy of the representation of a real number stored in a computer is determined by the precision of the mantissa.
- The error occurred due to the mantissa precision is the ***round-off error.***
- The actual number that is stored in the computer may be **chopping** or **rounding** of the last digit.
- The computer hardware works with a limited number of digits in machine numbers, errors are introduced and **propagated** in successive computations.

Chopping Off versus Rounding Off

Example:
Consider p expressed in *normalized decimal form*:

$$p = \pm 0.d_1 d_2 d_3 \cdots d_k d_{k+1} \cdots \times 10^n,$$

where $1 \leq d_1 \leq 9$ and $0 \leq d_j \leq 9$ for $j > 1$.

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If k is the maximum number of decimal digits; then the real number p is represented by $fl_{chop}(p)$, which is given by

$$fl_{chop}(p) = \pm 0.d_1 d_2 d_3 \cdots d_k \times 10^n, \tag{9}$$

Where $1 \leq d_1 \leq 9$ and $0 \leq d_j \leq 9$ for $1 < j \leq k$. The number $fl_{chop}(p)$ is called the ***chopped floating-point representation*** of p.

Chopping Off versus Rounding Off

On the other hand, the ***rounded floating-point representation*** $fl_{round}(p)$ is given by

$$fl_{round}(p) = \pm 0.d_1 d_2 d_3 \cdots r_k \times 10^n, \tag{10}$$

where $1 \leq d_1 \leq 9$ and $0 \leq d_j \leq 9$ for $1 < j < k$ and the last digit, r_k, is obtained by rounding the number $d_k d_{k+1} d_{k+2} \cdots$ to the nearest integer.

Chopping Off versus Rounding Off

Example:

The real number $p = \frac{22}{7} = 3.14285714285714285...$ has the following six-digit representations:

$$fl_{chop}(p) = 0.314285 \times 10^1,$$
$$fl_{round}(p) = 0.314286 \times 10^1.$$

For common purposes the chopping and rounding would be written as 3.14285 and 3.14286, respectively.

Contents

Loss of Significance

- Consider $p = 3.14155926536$ ans $q = 3.1415957341$, which are nearly equal and both carry 11 decimal digits of precision.
- Their difference is formed: $p - q = -0,0000030805$. Since the first six digits of p and q are the same, their difference $p - q$ contains only five decimal digits of precision.
- This phenomenon is called ***loss of significance***.

Loss of Significance

Example:

Compare the results of calculating $f(500)$ and $g(500)$ using six digits and rounding. Where, $f(x) = x(\sqrt{x+1} - \sqrt{x})$ and $g(x) = \dfrac{x}{\sqrt{x+1} + \sqrt{x}}$.

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For the first function,

$$f(500) = 500\left(\sqrt{501} - \sqrt{500}\right)$$

$$500(22.3830 - 22.3607) = 500(0.0223) = 11.1500$$

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$$g(500) = \frac{500}{\sqrt{501} + \sqrt{500}}$$

$$\frac{500}{22.3830 + 22.3607} = \frac{500}{44.7437} = 11.1748.$$

The second function, $g(x)$, is algebraically equivalent to $f(x)$, but the answer, $g(500) = 11.1748$, involves less error and it is the same as that obtained by rounding the true $11.17475300747198...$ to six digits.

Loss of Significance

Example: Compare the results of calculating $f(0.01)$ and $P(0.01)$ using six digits and rounding, where

$$f(x) = \frac{e^x - 1 - x}{x^2} \qquad \text{and} \qquad P(x) = \frac{1}{2} + \frac{x}{6} + \frac{x^2}{24}$$

The function $P(x)$ is the Taylor polynomial of degree $n = 2$ for $f(x)$ expanded about $x = 0$.

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For the first function

$$f(0.01) = \frac{e^{0.01} - 1 - 0.01}{(0.01)^2} = \frac{1.010050 - 1 - 0.01}{0.001} = 0.5.$$

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$$P(0.01) = \frac{1}{2} + \frac{0.01}{6} + \frac{0.001}{24} = 0.5 + 0.001667 + 0.000004 = 0.501671.$$

The answer $P(0.01) = 0.501671$ contains less error and it is the same as that obtained rounding the true answer $0.5016708416805\ldots$ to six digits.

Contents

$O(h^n)$ Order of Approximation

For functions

Definition 4.

The function $f(h)$ is said to be ***big Oh*** of $g(h)$, denoted $f(h) = \mathbf{O}(g(h))$, if there exist constants C and c such that:

$$|f(h)| \leq C|g(h)| \quad \text{whenever} \quad h \geq c. \tag{11}$$

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Example: Consider $f(x) = x^2 + 1$ and $g(x) = x^3$.

- Since $x^2 \leq x^3$ and $1 \leq x^3$ for $x \geq 1$
- it follows that $x^2 + 1 \leq 2x^3$ for $x \geq 1$.
- Therefore, $f(x) = \mathbf{O}(g(x))$, whenever $h \geq 1$.

The big Oh notation provides an useful way of describing the rate of growth of a function in terms of the well-known elementary function (x^n, $x^{1/n}$, a^x, $log_a(x), etc.$).

$O(h^n)$ Order of Approximation

For sequences

Definition 5.

Let $x_n = 1^\infty$ and $y_n = 1^\infty$ be two sequences. The sequence x_n is said to be of order big Oh of y_n, denoted $x_n = \mathbf{O}(y_n)$, if there exist constants C and N such that

$$|x_n| \leq C|y_n| \quad \text{whenever} \quad n \geq N. \tag{12}$$

$O(h^n)$ Order of Approximation

For sequences

Definition 5.

Let $x_n = 1^\infty$ and $y_n = 1^\infty$ be two sequences. The sequence x_n is said to be of order big Oh of y_n, denoted $x_n = \mathbf{O}(y_n)$, if there exist constants C and N such that

$$|x_n| \leq C|y_n| \quad \text{whenever} \quad n \geq N. \tag{12}$$

Example:

$\frac{n^2-1}{n^3} = \mathbf{O}\left(\frac{1}{n}\right)$, since $\frac{n^2-1}{n^3} \leq \frac{n^2}{n^3} = \frac{1}{n}$ whenever $n \geq 1$.

$O(h^n)$ Order of Approximation

Definition 6.

Assume that $f(h)$ is approximated by the function $p(h)$ and there exist a real constant $M > 0$ and a positive integer n so that

$$\frac{|f(h) - p(h)|}{h^n} \leq M \quad \text{for sufficiently small } h. \tag{13}$$

We say that $p(h)$ ***approximates*** $f(h)$ with order of approximation $\mathbf{O}(h^n)$ and write

$$f(h) = p(h) + \mathbf{O}(h^n) \tag{14}$$

When relation (13) is rewritten in the form $|f(h) - p(h)| \leq M|h^n|$, we see that the notation $\mathbf{O}(h^n)$ stands in place of the error bound $M|h^n|$.

$O(h^n)$ Order of Approximation

Theorem 2. Order of approximation for basic operations

Assume that $f(h) = p(h) + \mathbf{O}(h^n), g(h) = q(h) + \mathbf{O}(h^m)$, and $r = \min(m, n)$. Then

$$f(h) + g(h) = p(h) + q(h) + \mathbf{O}(h^r), \tag{15}$$

$$f(h)g(h) = p(h)q(h) + \mathbf{O}(h^r), \tag{16}$$

and

$$\frac{f(h)}{g(h)} = \frac{p(h)}{q(h)} + \mathbf{O}(h^r) \quad \text{provided that } g(h) \neq 0 \text{ and } q(h) \neq 0. \tag{17}$$

$O(h^n)$ Order of Approximation

Theorem 3. (Taylor's Theorem).

Assume $f \in C^{n+1}[a,b]$. If both x_0 and $x = x_0 + h$ lie in $[a,b]$, then

$$f(x_0 + h) = \sum_{k=0}^{n} \frac{f^{(k)}(x_0)}{k!} h^k + \mathbf{O}(h^{n+1}). \tag{18}$$

Additional properties:

(i) $\mathbf{O}(h^p) + \mathbf{O}(h^p) = \mathbf{O}(h^p)$,

(ii) $\mathbf{O}(h^p) + \mathbf{O}(h^q) = \mathbf{O}(h^r)$, where $r = \min(m,n)$, and

(iii) $\mathbf{O}(h^p)\mathbf{O}(h^q) = \mathbf{O}(h^s)$, where $s = p + q$.

$O(h^n)$ Order of Approximation

Example:
Consider the Taylor polynomial expansions

$$e^h = 1+h+\frac{h^2}{2!}+\frac{h^3}{3!}+\mathbf{O}(h^4) \qquad \text{and} \qquad \cos(h) = 1 - \frac{h^2}{2!} + \frac{h^4}{4!} + \mathbf{O}(h^6).$$

Determine the order of approximation for their sum and product.

$O(h^n)$ Order of Approximation

Example:
Consider the Taylor polynomial expansions

$$e^h = 1+h+\frac{h^2}{2!}+\frac{h^3}{3!}+\mathbf{O}(h^4) \qquad \text{and} \qquad \cos(h) = 1-\frac{h^2}{2!}+\frac{h^4}{4!}+\mathbf{O}(h^6).$$

Determine the order of approximation for their sum and product.

- For the sum we have

$$\begin{aligned} e^h+\cos(h) &= 1+h+\frac{h^2}{2!}+\frac{h^3}{3!}+\mathbf{O}(h^4)+1-\frac{h^2}{2!}+\frac{h^4}{4!}+\mathbf{O}(h^6) \\ &= 2+h+\frac{h^3}{3!}+\mathbf{O}(h^4)+\frac{h^4}{4!}+\mathbf{O}(h^6) \end{aligned}$$

$O(h^n)$ Order of Approximation

Since $\mathbf{O}(h^4) + \frac{h^4}{4!} = \mathbf{O}(h^4)$ and $\mathbf{O}(h^4) + \mathbf{O}(h^6) = \mathbf{O}(h^4)$, this reduces to

$$e^h + \cos(h) = 2 + h + \frac{h^3}{3!} + \mathbf{O}(h^4),$$

and the order of approximation is $\mathbf{O}(h^4)$.

$O(h^n)$ Order of Approximation

- The product is treated similarly:

$$
\begin{aligned}
e^h\cos(h) &= \left(1+h+\frac{h^2}{2!}+\frac{h^3}{3!}+\mathbf{O}(h^4)\right)\left(1-\frac{h^2}{2!}+\frac{h^4}{4!}+\mathbf{O}(h^6)\right)\\
&= \left(1+h+\frac{h^2}{2!}+\frac{h^3}{3!}\right)\left(1-\frac{h^2}{2!}+\frac{h^4}{4!}\right)+\\
&\quad \left(1+h+\frac{h^2}{2!}+\frac{h^3}{3!}\right)\mathbf{O}(h^6)+\left(1-\frac{h^2}{2!}+\frac{h^4}{4!}\right)\mathbf{O}(h^4)+\mathbf{O}(h^4)\mathbf{O}(h^6)\\
&= 1+h-\frac{h^3}{3}-\frac{5h^4}{24}-\frac{h^5}{24}+\frac{h^6}{48}+\frac{h^7}{144}+\mathbf{O}(h^6)+\mathbf{O}(h^4)+\mathbf{O}(h^4)\mathbf{O}(h^6).
\end{aligned}
$$

$O(h^n)$ Order of Approximation

Since $\mathbf{O}(h^4)\mathbf{O}(h^6) = \mathbf{O}(h^{10})$ and

$$\frac{-5h^4}{24} - \frac{h^5}{24} + \frac{h^6}{48} + \frac{h^7}{144} + \mathbf{O}(h^6) + \mathbf{O}(h^4) + \mathbf{O}(h^{10})$$

Since $\mathbf{O}(h^0) + \mathbf{O}(h^4) + \mathbf{O}(h^{10}) = \mathbf{O}(h^4)$, the preceding equation is simplified to yield

$$e^h \cos(h) = 1 + h + \frac{h^3}{3} + \mathbf{O}(h^4),$$

and the order of approximation is $\mathbf{O}(h^4)$.

Order of Convergence of a Sequence

Convergence of a sequence

Definition 7.

Suppose that $\lim_{n\longrightarrow\infty} x_n = x$ and $\{r_n\}_{n=1}^{\infty}$ is a sequence with $\lim_{n\longrightarrow\infty} r_n = 0$. We say that $\{x_n\}_{n=1}^{\infty}$ ***converges*** to x with the order of convergence $\mathbf{O}(r_n)$, if there exists a constant $K \geq 0$ such that

$$\frac{|x_n - x|}{|r_n|} \leq K \quad \text{for } n \text{ sufficiently large.} \tag{19}$$

This is indicated by writing $x_n = x + \mathbf{O}(\mathbf{r_n})$, or $x_n \longrightarrow x$ with order of convergence $\mathbf{O}(r_n)$

Order of Convergence of a Sequence

Definition 7.

Example:

Let $x_n = \cos(n)/n^2$ and $r_n = 1/n^2$ then,

$$\lim_{n \longrightarrow \infty} x_n = 0$$

with a rate of convergence $\mathrm{O}(1/n^2)$. This follows immediately from the relation

$$\frac{|\cos(n)/n^2|}{|1/n^2|} = |\cos(n) \leq 1| \text{ for all } n.$$

Contents

Propagation of Error

- **Addition** consider two numbers p and q (the true values) with the approximate values $\widehat{p}$ and $\widehat{q}$, which contains errors ϵ_p and ϵ_q, respectively. Starting with $p = \widehat{p} + \epsilon_p$ and $q = \widehat{q} + \epsilon_q$, the sum is

$$p + q = (\widehat{p} + \epsilon_p) + (\widehat{q} + \epsilon_q) = (\widehat{p} + \widehat{q}) + (\epsilon_p + \epsilon_q). \tag{20}$$

- Hence, for addition, the error in the sum is the **sum** of the errors in the addends.

$$\epsilon_s = \epsilon_p + \epsilon_q.$$

Propagation of Error

The propagation of error in **multiplication** is more complicated. The product is

$$pq = (\widehat{p} + \epsilon_p)(\widehat{q} + \epsilon_q) = \widehat{p}\widehat{q} + \widehat{p}\epsilon_p + \widehat{q}\epsilon_p + \epsilon_p\epsilon_q. \tag{21}$$

Propagation of Error

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Hence, if $\widehat{p}$ and $\widehat{q}$ are larger than 1 in absolute value, the terms $\widehat{p}\epsilon_q$ and $\widehat{q}\epsilon_p$ show that there is a possibility of magnification of the original errors ϵ_p and ϵ_q. Insights are gained if we look at the relative error. Rearrange the terms in (21) to get

$$pq - \widehat{p}\widehat{q} = \widehat{p}\epsilon_q + \widehat{q}\epsilon_p + \epsilon_p\epsilon_q. \tag{22}$$

Propagation of Error

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$$pq - \widehat{p}\widehat{q} = \widehat{p}\epsilon_q + \widehat{q}\epsilon_p + \epsilon_p\epsilon_q. \tag{22}$$

Suppose that $\widehat{p} \neq 0$ and $\widehat{q} \neq 0$; then we can divide (22) by pq to obtain the relative error in the product pq:

$$R_{pq} = \frac{pq - \widehat{p}\widehat{q}}{pq} = \frac{\widehat{p}\epsilon_q + \widehat{q}\epsilon_p + \epsilon_p\epsilon_q}{pq} = \frac{\widehat{p}\epsilon_q}{pq} + \frac{\widehat{q}\epsilon_p}{pq} + \frac{\epsilon_p\epsilon_q}{pq}. \tag{23}$$

Propagation of Error

Furthermore, suppose that $\widehat{p}$ and $\widehat{q}$ are good approximations for $\widehat{p}$ and $\widehat{q}$; then $\widehat{p}/p \approx 1, \widehat{q}/q \approx 1$, and $R_p R_q = (\epsilon_p/p)(\epsilon_q/q) \approx 0$ (R_p and R_q are the relative errors in the approximations $\widehat{p}$ and $\widehat{q}$). Then making these substitutions yields the simplified relationship

$$R_{pq} = \frac{pq - \widehat{p}\widehat{q}}{pq} \approx \epsilon_q/q + \epsilon_p/p + 0 = R_q + R_p. \tag{24}$$

Propagation of Error

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$$R_{pq} = \frac{pq - \widehat{p}\widehat{q}}{pq} \approx \epsilon_q/q + \epsilon_p/p + 0 = R_q + R_p. \tag{24}$$

This shows that the relative error in the product $\mathbf{pq}$ is approximately **the sum of the relative errors** in the approximations $\widehat{\mathbf{p}}$ and $\widehat{\mathbf{q}}$.

A quality that is desirable for any numerical process is that a small error in the initial conditions will produce small changes in the final result. An algorithm with this feature is called ***stable;*** otherwise, it is called ***unstable***.

Propagation of Error

Definition 8.

Suppose that ϵ represents an initial error and $\epsilon(n)$ represents the growth of the error after n steps. If $|\epsilon(n)| \approx n\epsilon$, the growth of error is said to be ***linear***. If $|\epsilon(n)| \approx K^n\epsilon$, the growth of error is called ***exponential***. If $K > 1$, the exponential error growns without bound as $n \longrightarrow \infty$, and if $0 < K < 1$, the exponential error diminishes to zero as $n \longrightarrow \infty$.

Propagation of error

Example: Show that the following three schemes can be used with finite-precision arithmetic to recursively generate the terms in the sequence $\{1/3^n\}_{n=0}^{\infty}$.

$$r_0 = 1 \quad \text{and} \quad r_n = \frac{1}{3} r_{n-1} \quad \text{for} \quad n = 1, 2, \cdots, \tag{25}$$

$$p_0 = 1, p_1 = \frac{1}{3}, \quad \text{and} \quad p_n = \frac{4}{3} p_{n-1} - \frac{1}{3} p_{n-2} \quad \text{for} \quad n = 1, 2, \cdots, \tag{26}$$

$$q_0 = 1, q_1 = \frac{1}{3}, \quad \text{and} \quad q_n = \frac{10}{3} q_{n-1} - q_{n-2} \quad \text{for} \quad n = 1, 2, \cdots, \tag{27}$$

Propagation of error

Formula (25) is obvious. In (26) the difference equation has the general solution $p_n = A(1/3^n) + B$. This can be verified by direct substitution:

$$\begin{aligned}\frac{4}{3}p_{n-1} - \frac{1}{3}p_{n-2} &= \frac{4}{3}\left(\frac{A}{3^{n-1}} + B\right) - \frac{1}{3}\left(\frac{A}{3^{n-2}} + B\right) \\ &= \left(\frac{4}{3^n} - \frac{3}{3^n}\right)A - \left(\frac{4}{3} - \frac{1}{3}\right)B = A\frac{1}{3^n} + B = p_n\end{aligned}$$

Setting $A = 1$ and $B = 0$ will generate the sequence desired.

Propagation of error

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Setting $A = 1$ and $B = 0$ will generate the sequence desired. In (27) the difference equation has the general solution $q_n = A(1/3^n) + B3^n$. This too verified by substitution:

$$\begin{aligned}\frac{10}{3}q_{n-1} - q_{n-2} &= \frac{10}{3}\left(\frac{A}{3^{n-1}} + B3^{n-1}\right) - \left(\frac{A}{3^{n-2}} + B3^{n-2}\right) \\ &= \left(\frac{10}{3^n} - \frac{9}{3^n}\right)A - (10-1)3^{n-1}B = A\frac{1}{3^n} + B3^n = q_n\end{aligned}$$

Propagation of error

Example:
Generate approximations to the sequences $\{x_n\} = 1/3^n$ using hemes

$$r_0 = 0.99996 \quad \text{and} \quad r_n = \frac{1}{3} r_{n-1} \quad \text{for} \quad n = 1, 2, \cdots, \tag{28}$$

$$p_0 = 1, p_1 = 0.33332, \quad \text{and} \quad p_n = \frac{4}{3} p_{n-1} - \frac{1}{3} p_{n-2} \quad \text{for} \quad n = 1, 2, \cdots, \tag{29}$$

$$q_0 = 1, q_1 = 0.33332, \quad \text{and} \quad q_n = \frac{10}{3} p_{n-1} - p_{n-2} \quad \text{for} \quad n = 1, 2, \cdots, \tag{30}$$

In (28) the initial error in r_0 is 0.00004, and in (29) and (30) the initial errors in p_1 and q_1 are 0.000013. Investigate the propagation of error for each scheme.

Propagation of error

Table: Sequence $x_n = 1/3^n$ and the approximations r_n, p_n, and q_n

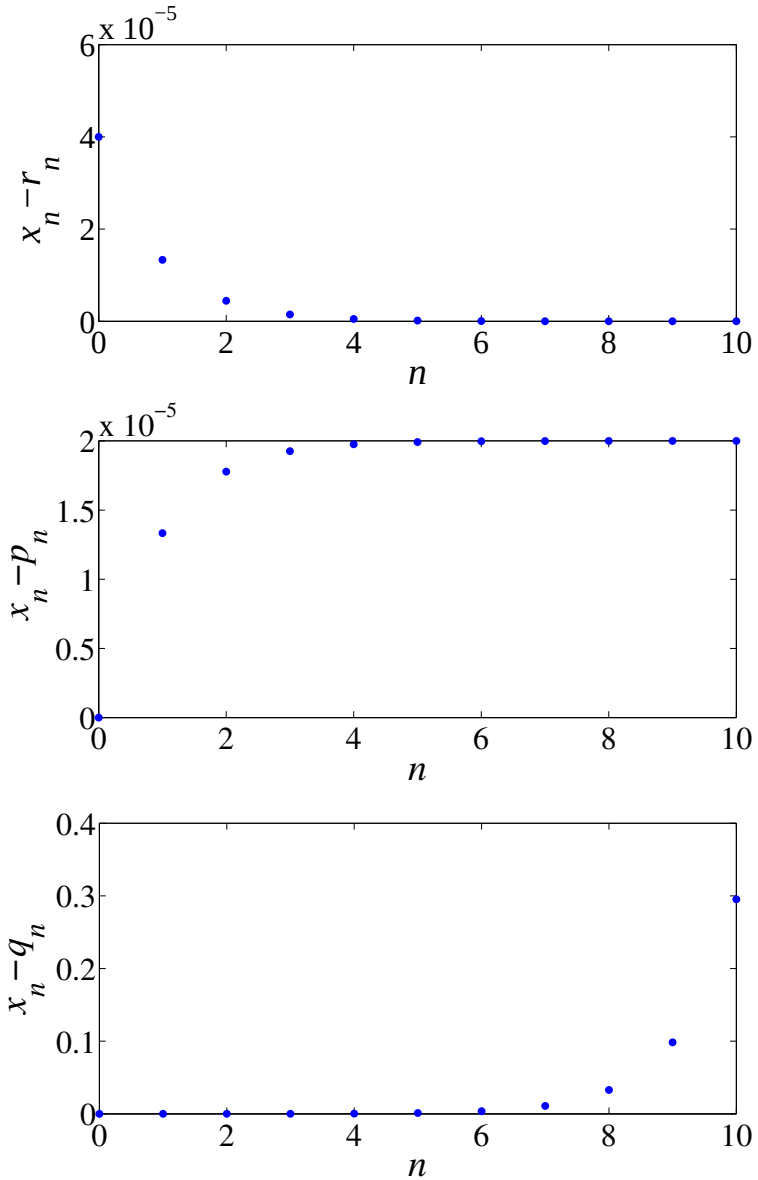
n	x_n	r_n	p_n	q_n
0	1.0000000000	0.9999600000	1.0000000000	1.0000000000
1	0.3333333333	0.3333200000	0.3333200000	0.3333200000
2	0.1111111111	0.1111066667	0.1110933333	0.1110666667
3	0.0370370370	0.0370355556	0.0370177778	0.0369022222
4	0.0123456790	0.0123451852	0.0123259259	0.0119407407
5	0.0041152263	0.0041150617	0.0040953086	0.0029002469
6	0.0013717421	0.0013716872	0.0013517695	-0.0022732510
7	0.0004572474	0.0004572291	0.0004372565	-0.0104777503
8	0.0001524158	0.0001524097	0.0001324188	-0.0326525834
9	0.0000508053	0.0000508032	0.0000308063	-0.0983641945
10	0.0000169351	0.0000169344	-0.0000030646	-0.2952280648

Propagation of error

Table: Error sequences $x_n - r_n$, $x_n - p_n$, and $x_n - q_n$

n	$x_n - r_n$	$x_n - p_n$	$x_n - q_n$
0	0.0000400000	0.0000000000	0.0000000000
1	0.0000133333	0.0000133333	0.0000133333
2	0.0000044444	0.0000177778	0.0000444444
3	0.0000014815	0.0000192593	0.0001348148
4	0.0000004938	0.0000197531	0.0004049383
5	0.0000001646	0.0000199177	0.0012149794
6	0.0000000549	0.0000199726	0.0036449931
7	0.0000000183	0.0000199909	0.0109349977
8	0.0000000061	0.0000199970	0.0328049992
9	0.0000000020	0.0000199990	0.0984149997
10	0.0000000007	0.0000199997	0.2952449999

Propagation of error



- The error for $\{r_n\}$ is stable and decreases in an exponential manner.
- The error $\{p_n\}$ is stable.
- The error for $\{q_n\}$ is unstable and grows at an exponential rate.

Although the error for $\{p_n\}$ is stable, the terms $p_n \longrightarrow 0$ as $n \longrightarrow \infty$, so that the error eventually dominates and the terms past p_8 have no significant digits.