Mathematical preliminaries and error analysis

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September 21, 2014

Outline

1. **Round-off errors and computer arithmetic**
   - IEEE standard floating-point format
   - Absolute and Relative Errors
   - Machine Epsilon
   - Loss of Significance
2. **Algorithms and Convergence**
   - Algorithm
   - Stability
   - Rate of convergence

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What is the difference for the arithmetic in algebra and computer?

1. For arithmetic in algebra,

$$256 + 1 = 257, \quad \left(\sqrt{256+1}\right)^2 = 257$$

2. For arithmetic in computer (MATLAB),
   - int8(256) + int8(1) = 127 ???????
   - int16(256) + int16(1) = 257
   - sqrt(256+1)ˆ2 = ? The solution is equal to 257 or not.
   - (single(sqrt(5))+single(sqrt(3)))ˆ2 - (sqrt(3)+sqrt(5))ˆ2

Example 1

Consider the following recurrence algorithm

$$\begin{cases} x_0 = 1, \qquad x_1 = \frac{1}{3} \\ x_{n+1} = \frac{13}{3} x_n - \frac{4}{3} x_{n-1} \end{cases}$$

for computing the sequence of $\{x_n = (\frac{1}{3})^n\}$.

Matlab program

```
n = 30; x = zeros(n,1); x(1) = 1; x(2) = 1/3;
for ii = 3:n
    x(ii) = 13 / 3 * x(ii-1) - 4 / 3 * x(ii-2);
    xn = (1/3)^(ii-1);    RelErr = abs(xn-x(ii)) / xn;
    fprintf('x(%2.0f) = %15.8e, x_ast(%2.0f) = %14.8e,', ...
        'RelErr(%2.0f) = %11.4e \n', ii,x(ii),ii,xn,ii,RelErr);
end
```

Example 2

What is the binary representation of $\frac{2}{3}$?

Solution: To determine the binary representation for $\frac{2}{3}$, we write

$$\frac{2}{3} = (0.a_1a_2a_3\dots)_2.$$

Multiply by 2 to obtain

$$\frac{4}{3} = (a_1.a_2a_3\dots)_2.$$

Therefore, we get $a_1 = 1$ by taking the integer part of both sides.

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Subtracting 1, we have

$$\frac{1}{3} = (0.a_2a_3a_4\ldots)_2.$$

Repeating the previous step, we arrive at

$$\frac{2}{3} = (0.101010\ldots)_2.$$

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- In the computational world, each representable number has only a fixed and finite number of digits.
- For any real number x, let

$$x = \pm 1.a_1 a_2 \cdots a_t a_{t+1} a_{t+2} \cdots \times 2^m,$$

denote the normalized scientific binary representation of x.

- In 1985, the IEEE (Institute for Electrical and Electronic Engineers) published a report called *Binary Floating Point Arithmetic Standard 754-1985*. In this report, formats were specified for single, double, and extended precisions, and these standards are generally followed by microcomputer manufactures using floating-point hardware.

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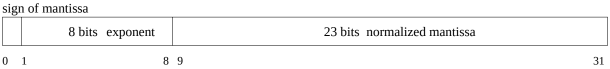
Single precision

- The single precision IEEE standard floating-point format allocates 32 bits for the normalized floating-point number $\pm q \times 2^m$ as shown in the following figure.



- The first bit is a sign indicator, denoted s. This is followed by an 8-bit exponent c and a 23-bit mantissa f.
- The base for the exponent and mantissa is 2, and the actual exponent is $c - 127$. The value of c is restricted by the inequality $0 \leq c \leq 255$.

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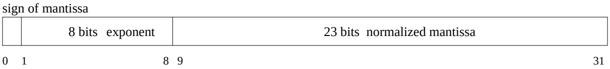

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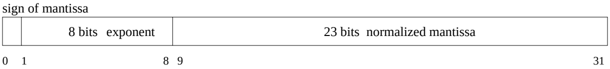

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- A normalization is imposed that requires that the leading digit in fraction be 1, and this digit is not stored as part of the 23-bit mantissa.
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Example 3

What is the decimal number of the machine number

$$0\underline{10000001}01000000000000000000000?$$

1. The leftmost bit is zero, which indicates that the number is positive.
2. The next 8 bits, 10000001, are equivalent to

   $$c = 1 \cdot 2^7 + 0 \cdot 2^6 + \cdots + 0 \cdot 2^1 + 1 \cdot 2^0 = 129.$$

   The exponential part of the number is $2^{129-127} = 2^2$.
3. The final 23 bits specify that the mantissa is

   $$f = 0 \cdot (2)^{-1} + 1 \cdot (2)^{-2} + 0 \cdot (2)^{-3} + \cdots + 0 \cdot (2)^{-23} = 0.25.$$

4. Consequently, this machine number precisely represents the decimal number

   $$(-1)^s 2^{c-127}(1+f) = 2^2 \cdot (1 + 0.25) = 5.$$

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1. The final 23 bits specify that the mantissa is

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Summary

Above three examples

$$\begin{array}{lcl} 0\underline{10000001}00111111111111111111111 & \Rightarrow & 4.99999523162842 \\ 0\underline{10000001}01000000000000000000000 & \Rightarrow & 5 \\ 0\underline{10000001}01000000000000000000001 & \Rightarrow & 5.00000476837158 \end{array}$$

- Only a relatively small subset of the real number system is used for the representation of all the real numbers.
- This subset, which are called the *floating-point numbers*, contains only rational numbers, both positive and negative.
- When a number can not be represented exactly with the fixed finite number of digits in a computer, a near-by floating-point number is chosen for approximate representation.

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Above three examples

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The smallest positive number

Let $s = 0$, $c = 1$ and $f = 0$ which is equivalent to

$$2^{-126} \cdot (1 + 0) \approx 1.175 \times 10^{-38}$$

The largest number

Let $s = 0$, $c = 254$ and $f = 1 - 2^{-23}$ which is equivalent to

$$2^{127} \cdot (2 - 2^{-23}) \approx 3.403 \times 10^{38}$$

Definition 6

If a number x with $|x| < 2^{-126} \cdot (1 + 0)$, then we say that an *underflow* has occurred and is generally set to zero.
If $|x| > 2^{127} \cdot (2 - 2^{-23})$, then we say that an *overflow* has occurred.

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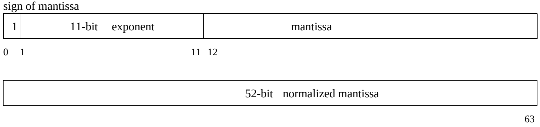
Double precision

- A floating point number in double precision IEEE standard format uses two words (64 bits) to store the number as shown in the following figure.



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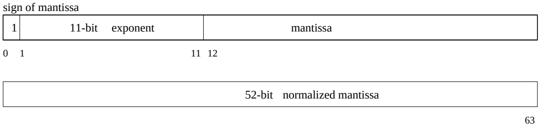

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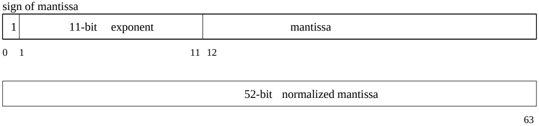

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Format of floating-point number

$$(-1)^s \times (1+f) \times 2^{c-1023}$$

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Chopping and rounding

For any real number x, let

$$x = \pm 1.a_1 a_2 \cdots a_t a_{t+1} a_{t+2} \cdots \times 2^m,$$

denote the normalized scientific binary representation of x.

1. **chopping:** simply discard the excess bits $a_{t+1}, a_{t+2}, \ldots$ to obtain

$$fl(x) = \pm 1.a_1 a_2 \cdots a_t \times 2^m.$$

2. **rounding:** add $2^{-(t+1)} \times 2^m$ to x and then chop the excess bits to obtain a number of the form

$$fl(x) = \pm 1.\delta_1 \delta_2 \cdots \delta_t \times 2^m.$$

In this method, if $a_{t+1} = 1$, we add 1 to a_t to obtain $fl(x)$, and if $a_{t+1} = 0$, we merely chop off all but the first t digits.

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Definition 7 (Roundoff error)

The error results from replacing a number with its floating-point form is called *roundoff error* or *rounding error*.

Definition 8 (Absolute Error and Relative Error)

If x is an approximation to the exact value x^*, the absolute error is $|x^* - x|$ and the relative error is $\frac{|x^*-x|}{|x^*|}$, provided that $x^* \neq 0$.

Example 9

(a) If $x^* = 0.3000 \times 10^{-3}$ and $x = 0.3100 \times 10^{-3}$, then the absolute error is 0.1×10^{-4} and the relative error is 0.3333×10^{-1}.
(b) If $x^* = 0.3000 \times 10^{4}$ and $x = 0.3100 \times 10^{4}$, then the absolute error is 0.1×10^{3} and the relative error is 0.3333×10^{-1}.

Definition 7 (Roundoff error)

The error results from replacing a number with its floating-point form is called *roundoff error* or *rounding error*.

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If x is an approximation to the exact value x^*, the absolute error is $|x^* - x|$ and the relative error is $\frac{|x^*-x|}{|x^*|}$, provided that $x^* \neq 0$.

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As a measure of accuracy, the absolute error may be misleading and the relative error more meaningful.

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The number x is said to approximate x^* to t significant digits if t is the largest nonnegative integer for which

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- If the floating-point representation $fl(x)$ for the number x is obtained by using t digits and chopping procedure, then the relative error is

$$\frac{|x - fl(x)|}{|x|} = \frac{|0.00\cdots 0a_{t+1}a_{t+2}\cdots \times 2^m|}{|1.a_1a_2\cdots a_ta_{t+1}a_{t+2}\cdots \times 2^m|} = \frac{|0.a_{t+1}a_{t+2}\cdots|}{|1.a_1a_2\cdots a_ta_{t+1}a_{t+2}\cdots|} \times 2^{-t}.$$

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  - $a_{t+1} = 0$, then $fl(x) = \pm 1.a_1 a_2 \cdots a_t \times 2^m$. A bound for the relative error is

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Definition 11 (Machine epsilon)

The floating-point representation, $fl(x)$, of x can be expressed as

$$fl(x) = x(1+\delta), \quad |\delta| \le \varepsilon_M, \tag{1}$$

where $\varepsilon_M \equiv 2^{-t}$ is referred to as the *unit roundoff error* or *machine epsilon*.

Single precision IEEE standard floating-point format

The mantissa f corresponds to 23 binary digits (i.e., $t = 23$), the machine epsilon is

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which provides between 15 and 16 decimal digits of accuracy.

Summary of IEEE standard floating-point format

	single precision	double precision
ε_M	1.192×10^{-7}	2.220×10^{-16}
smallest positive number	1.175×10^{-38}	2.225×10^{-308}
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- Whenever two machine numbers x and y are to be combined arithmetically, the computer will produce $fl(x \odot y)$ instead of $x \odot y$.
- Under (1), the relative error of $fl(x \odot y)$ satisfies

$$fl(x \odot y) = (x \odot y)(1 + \delta), \quad \delta \leq \varepsilon_M, \tag{2}$$

  where ε_M is the unit roundoff.
- But if x, y are not machine numbers, then they must first rounded to floating-point format before the arithmetic operation and the resulting relative error becomes

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Example

Let $x = 0.54617$ and $y = 0.54601$. Using rounding and four-digit arithmetic, then

- $x^* = fl(x) = 0.5462$ is accurate to four significant digits since

$$\frac{|x - x^*|}{|x|} = \frac{0.00003}{0.54617} = 5.5 \times 10^{-5} \le 5 \times 10^{-4}.$$

- $y^* = fl(y) = 0.5460$ is accurate to five significant digits since

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But

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Since

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- One of the most common error-producing calculations involves the cancellation of significant digits due to the subtraction of nearly equal numbers or the addition of one very large number and one very small number.
- Sometimes, loss of significance can be avoided by rewriting the mathematical formula.

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The quadratic formulas for computing the roots of $ax^2 + bx + c = 0$, when $a \neq 0$, are

$$x_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad \text{and} \quad x_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}.$$

Consider the quadratic equation $x^2 + 62.10x + 1 = 0$ and discuss the numerical results.

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Solution

- Using the quadratic formula and 8-digit rounding arithmetic, one can obtain

$$x_1 = -0.01610723 \qquad \text{and} \qquad x_2 = -62.08390.$$

- Now we perform the calculations with 4-digit rounding arithmetic. First we have

$$\sqrt{b^2 - 4ac} = \sqrt{62.10^2 - 4.000} = \sqrt{3856 - 4.000} = 62.06,$$

and

$$fl(x_1) = \frac{-62.10 + 62.06}{2.000} = \frac{-0.04000}{2.000} = -0.02000.$$

The relative error in computing x_1 is

$$\frac{|fl(x_1) - x_1|}{|x_1|} = \frac{|-0.02000 + 0.01610723|}{|-0.01610723|} \approx 0.2417 \leq 5 \times 10$$

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$$fl(x_2) = \frac{-62.10 - 62.06}{2.000} = \frac{-124.2}{2.000} = -62.10,$$

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$$\frac{|fl(x_2) - x_2|}{|x_2|} = \frac{|-62.10 + 62.08390|}{|-62.08390|} \approx 0.259\times 10^{-3} \le 5\times 10^{-4}.$$

- In this equation, $b^2 = 62.10^2$ is much larger than $4ac = 4$. Hence b and $\sqrt{b^2 - 4ac}$ become two nearly equal numbers. The calculation of x_1 involves the subtraction of two nearly equal numbers.
- To obtain a more accurate 4-digit rounding approximation for x_1, we change the formulation by rationalizing the numerator, that is,

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- In this equation, $b^2 = 62.10^2$ is much larger than $4ac = 4$. Hence b and $\sqrt{b^2 - 4ac}$ become two nearly equal numbers. The calculation of x_1 involves the subtraction of two nearly equal numbers.
- To obtain a more accurate 4-digit rounding approximation for x_1, we change the formulation by rationalizing the numerator, that is,

$$x_1 = \frac{-2c}{b + \sqrt{b^2 - 4ac}}.$$

- In calculating x_2,

$$fl(x_2) = \frac{-62.10 - 62.06}{2.000} = \frac{-124.2}{2.000} = -62.10,$$

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Then

$$fl(x_1) = \frac{-2.000}{62.10 + 62.06} = \frac{-2.000}{124.2} = -0.01610.$$

The relative error in computing x_1 is now reduced to 6.2×10^{-4} ∎

Example 13

Let

$$\begin{aligned} p(x) &= x^3 - 3x^2 + 3x - 1, \\ q(x) &= ((x-3)x+3)x - 1. \end{aligned}$$

Compare the function values at $x = 2.19$ with using three-digit arithmetic.

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Compare the function values at $x = 2.19$ with using three-digit arithmetic.

Solution

Use 3-digit and rounding for $p(2.19)$ and $q(2.19)$.

$$\begin{aligned}
\hat{p}(2.19) &= ((2.19^3 - 3 \times 2.19^2) + 3 \times 2.19) - 1 \\
&= ((10.5 - 14.4) + 3 \times 2.19) - 1 \\
&= (-3.9 + 6.57) - 1 \\
&= 2.67 - 1 = 1.67
\end{aligned}$$

and

$$\begin{aligned}
\hat{q}(2.19) &= ((2.19 - 3) \times 2.19 + 3) \times 2.19 - 1 \\
&= (-0.81 \times 2.19 + 3) \times 2.19 - 1 \\
&= (-1.77 + 3) \times 2.19 - 1 \\
&= 1.23 \times 2.19 - 1 \\
&= 2.69 - 1 = 1.69.
\end{aligned}$$

With more digits, one can have

$$p(2.19) = g(2.19) = 1.685159$$

Hence the absolute errors are

$$|p(2.19) - \hat{p}(2.19)| = 0.015159$$

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Exercise

Page 28: 4, 11, 12, 15, 18

Definition 14 (Algorithm)

An algorithm is a procedure that describes a finite sequence of steps to be performed in a specified order.

Example 15

Give an algorithm to compute $\sum_{i=1}^{n} x_i$, where n and $x_1, x_2, \ldots, x_n$ are given.

Algorithm

INPUT	$n, x_1, x_2, \ldots, x_n$.
OUTPUT	$SUM = \sum_{i=1}^{n} x_i$.
Step 1.	Set $SUM = 0$. (Initialize accumulator.)
Step 2.	For $i = 1, 2, \ldots, n$ do
	Set $SUM = SUM + x_i$. (Add the next term.)
Step 3.	OUTPUT SUM;
	STOP

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Definition 16 (Stable)

An algorithm is called stable if small changes in the initial data of the algorithm produce correspondingly small changes in the final results.

Definition 17 (Unstable)

An algorithm is unstable if small errors made at one stage of the algorithm are magnified and propagated in subsequent stages and seriously degrade the accuracy of the overall calculation.

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Whether an algorithm is stable or unstable should be decided on the basis of relative error.

Example 18

Consider the following recurrence algorithm

$$\begin{cases} x_0 = 1, \qquad x_1 = \frac{1}{3} \\ x_{n+1} = \frac{13}{3} x_n - \frac{4}{3} x_{n-1} \end{cases}$$

for computing the sequence of $\{x_n = (\frac{1}{3})^n\}$. This algorithm is unstable.

A Matlab implementation of the recurrence algorithm gives the following result.

n	x_n	x_n^*	RelErr
8	4.57247371e-04	4.57247371e-04	4.4359e-10
10	5.08052602e-05	5.08052634e-05	6.3878e-08
12	5.64497734e-06	5.64502927e-06	9.1984e-06
14	6.26394672e-07	6.27225474e-07	1.3246e-03
15	2.05751947e-07	2.09075158e-07	1.5895e-02
16	5.63988754e-08	6.96917194e-08	1.9074e-01
17	-2.99408028e-08	2.32305731e-08	2.289e+00
20	-3.40210767e-06	8.60391597e-10	3.955e+03
23	-2.17789924e-04	3.18663555e-11	6.835e+06
27	-5.57542287e-02	3.93411796e-13	1.417e+11
30	-3.56827064e+00	1.45708072e-14	2.449e+14

For any constants c_1 and c_2,

$$x_n = c_1 \left(\frac{1}{3}\right)^n + c_2 \left(4^n\right)$$

is a solution to the recursive equation

$$x_n = \frac{13}{3} x_{n-1} - \frac{4}{3} x_{n-2}$$

since

$$\begin{aligned}
&\frac{13}{3} x_{n-1} - \frac{4}{3} x_{n-2} \\
&= \frac{13}{3} \left[c_1 \left(\frac{1}{3}\right)^{n-1} + c_2 4^{n-1} \right] - \frac{4}{3} \left[c_1 \left(\frac{1}{3}\right)^{n-2} + c_2 4^{n-2} \right] \\
&= c_1 \left(\frac{1}{3}\right)^{n-2} \left(\frac{13}{3} \cdot \frac{1}{3} - \frac{4}{3} \right) + c_2 4^{n-2} \left(\frac{13}{3} \cdot 4 - \frac{4}{3} \right) \\
&= c_1 \left(\frac{1}{3}\right)^n + c_2 4^n = x_n.
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&= c_1 \left(\frac{1}{3}\right)^{n-2}\left(\frac{13}{3}\cdot\frac{1}{3} - \frac{4}{3}\right) + c_2 4^{n-2}\left(\frac{13}{3}\cdot 4 - \frac{4}{3}\right) \\
&= c_1 \left(\frac{1}{3}\right)^{n} + c_2 4^{n} = x_n.
\end{aligned}$$

Take $x_0 = 1$ and $x_1 = \frac{1}{3}$. This determine unique values as $c_1 = 1$ and $c_2 = 0$. Therefore,

$$x_n = \left(\frac{1}{3}\right)^n \quad \text{for all } n.$$

In computer arithmetic, $\hat{x}_0 = 1$ and $\hat{x}_1 = 0.33\cdots3$. The generated sequence $\{\hat{x}_n\}$ is then given by

$$\hat{x}_n = \hat{c}_1 \left(\frac{1}{3}\right)^n + \hat{c}_2 \left(4^n\right),$$

where $\hat{c}_1 \approx 1$ and $|\hat{c}_2| \approx \varepsilon$. Therefore, the round-off error is

$$x_n - \hat{x}_n = (1 - \hat{c}_1) \left(\frac{1}{3}\right)^n - \hat{c}_2 \left(4^n\right)$$

which grows exponentially with n.

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Matlab program

```
n = 30;
x = zeros(n,1);
x(1) = 1;
x(2) = 1/3;
for ii = 3:n
    x(ii) = 13 / 3 * x(ii-1) - 4 / 3 * x(ii-2);
    xn = (1/3)^(ii-1);
    RelErr = abs(xn-x(ii)) / xn;
    fprintf('x(%2.0f) = %20.8d, x_ast(%2.0f) = %20.8d,', ...
        'RelErr(%2.0f) = %14.4d \n', ii,x(ii),ii,xn,ii,RelErr);
end
```

Example 19

Consider the following recurrence algorithm

$$\begin{cases} x_0 = 1, \qquad x_1 = \frac{1}{3} \\ x_{n+1} = 2x_n - x_{n-1} \end{cases}$$

for computing the sequence of $\{x_n = 1 - \frac{2}{3}n\}$. This algorithm is stable.

For any constants c_1 and c_2,

$$x_n = c_1 + c_2 n$$

is a solution to the recursive equation

$$x_n = 2x_{n-1} - x_{n-2}.$$

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Take $x_0 = 1$ and $x_1 = \frac{1}{3}$. This determine unique values as $c_1 = 1$ and $c_2 = -\frac{2}{3}$. Therefore,

$$x_n = 1 - \frac{2}{3}n, \quad \text{for all } n.$$

In computer arithmetic, $\hat{x}_0 = 1$ and $\hat{x}_1 = 0.33\cdots3$. The generated sequence $\{\hat{x}_n\}$ is then given by

$$\hat{x}_n = \hat{c}_1 - \hat{c}_2 n,$$

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$$x_n - \hat{x}_n = (1 - \hat{c}_1) - \left(\frac{2}{3} - \hat{c}_2\right) n$$

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Definition 20

Suppose $\{\beta_n\} \to 0$ and $\{x_n\} \to x^*$. If $\exists\ c > 0$ and an integer $N > 0$ such that

$$|x_n - x^*| \leq c|\beta_n|, \quad \forall\ n \geq N,$$

then we say $\{x_n\}$ converges to x^* with rate of convergence $O(\beta_n)$, and write $x_n = x^* + O(\beta_n)$.

Example 21

Compare the convergence behavior of $\{x_n\}$ and $\{y_n\}$, where

$$x_n = \frac{n+1}{n^2}, \quad \text{and} \quad y_n = \frac{n+3}{n^3}.$$

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$$x_n = \frac{n+1}{n^2}, \quad \text{and} \quad y_n = \frac{n+3}{n^3}.$$

Solution:

Note that both

$$\lim_{n\to\infty} x_n = 0 \quad \text{and} \quad \lim_{n\to\infty} y_n = 0.$$

Let $\alpha_n = \frac{1}{n}$ and $\beta_n = \frac{1}{n^2}$. Then

$$\begin{aligned} |x_n - 0| &= \frac{n+1}{n^2} \le \frac{n+n}{n^2} = \frac{2}{n} = 2\alpha_n, \\ |y_n - 0| &= \frac{n+3}{n^3} \le \frac{n+3n}{n^3} = \frac{4}{n^2} = 4\beta_n. \end{aligned}$$

Hence

$$x_n = 0 + O(\frac{1}{n}) \quad \text{and} \quad y_n = 0 + O(\frac{1}{n^2}).$$

This shows that $\{y_n\}$ converges to 0 much faster than $\{x_n\}$. ■

Exercise

Page 39: 3.a, 6, 7, 11