

# Mathematical Preliminaries and Error Analysis

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<sup>1</sup>These slides are based on Prof. Tsung-Ming Huang(NTNU)'s original slides A set of small navigation icons including arrows, a search icon, and a refresh icon.

# 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



# Terminologies

- binary: 二進位, decimal: 十進位, hexadecimal: 十六進位
- exponent: 指數, mantissa: 尾數
- floating point numbers: 浮點數
- chopping: 無條件捨去, rounding: 四捨五入(X捨Y入)
- single precision: 單精度, double precision: 雙精度
- round-off error: 捨入誤差
- significant digits: 有效位數
- loss of significance: 有效位數喪失





Subtracting 1, we have

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

Repeating the previous step, we arrive at

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



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

$$x = \pm 1.a_1a_2 \cdots a_t a_{t+1} a_{t+2} \cdots \times 2^m,$$

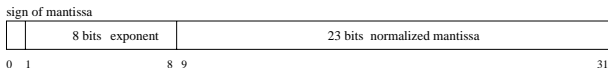
denote the normalized scientific binary representation of  $x$ .

- 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 to design floating-point hardware.



# 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  $s$ . It 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 to  $0 \leq c \leq 255$ .



- The actual exponent of the number is restricted to  $-127 \leq c - 127 \leq 128$ .
- A normalization is imposed so that the leading digit in fraction be 1, and this digit "1" is not stored as part of the 23-bit mantissa  $f$ .
- The resulting floating-point number takes the form

$$(-1)^s 2^{c-127} (1 + f).$$





## Example

What is the decimal number of the machine number

01000000101000000000000000000000000000000?

- 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 the mantissa:

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

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

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



**Example**

What is the decimal number of the machine number

01000000100111111111111111111111111111111?

- 1 The final 23 bits specify that the mantissa is

$$\begin{aligned} f &= 0 \cdot (2)^{-1} + 0 \cdot (2)^{-2} + 1 \cdot (2)^{-3} + \cdots + 1 \cdot (2)^{-23} \\ &= 0.2499998807907105. \end{aligned}$$

- 2 Consequently, this machine number precisely represents the decimal number

$$\begin{aligned} (-1)^s 2^{c-127} (1 + f) &= 2^2 \cdot (1 + 0.2499998807907105) \\ &= 4.999999523162842. \end{aligned}$$



**Example**

What is the decimal number of the machine number

010000001010000000000000000000001?

- 1 The final 23 bits specify that the mantissa is

$$\begin{aligned} f &= 0 \cdot 2^{-1} + 1 \cdot 2^{-2} + 0 \cdot 2^{-3} + \dots + 0 \cdot 2^{-22} + 1 \cdot 2^{-23} \\ &= 0.2500001192092896. \end{aligned}$$

- 2 Consequently, this machine number precisely represents the decimal number

$$\begin{aligned} (-1)^s 2^{c-127} (1 + f) &= 2^2 \cdot (1 + 0.2500001192092896) \\ &= 5.000000476837158. \end{aligned}$$



# Summary

## Above three examples

01000000100111111111111111111111111111111  $\Rightarrow$  4.999999523162842

01000000101000000000000000000000000000000  $\Rightarrow$  5

01000000101000000000000000000000000000001  $\Rightarrow$  5.000000476837158

- 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.



## The smallest (normalized) positive number

Let  $s = 0$ ,  $c = 1$  and  $f = 0$ . This corresponds 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

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

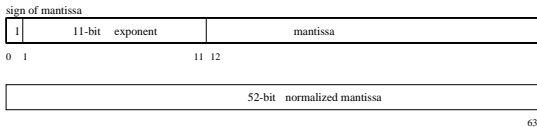
## Definition

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. It is sometimes referred to as an IEEE 'subnormal' or 'denormal' and corresponds to  $c = 0$ . If  $|x| > 2^{127} \cdot (2 - 2^{-23})$ , then we say that an *overflow* has occurred.



# 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.



- The **first** bit is a sign indicator, denoted  $s$ . It is followed by an **11-bit** exponent  $e$  and a **52-bit** mantissa  $f$ .
- The actual exponent is  $e - 1023$ .



## Format of floating-point number

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

## The smallest (normalized) positive number

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

$$2^{-1022} \cdot (1 + 0) \approx 2.225 \times 10^{-308}.$$

## The largest number

Let  $s = 0$ ,  $c = 2046$  and  $f = 1 - 2^{-52}$  which is equivalent to

$$2^{1023} \cdot (2 - 2^{-52}) \approx 1.798 \times 10^{308}.$$



# 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  $a_{t+1}, a_{t+2}, \dots$  to obtain

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

- 2 **rounding**: add  $\pm 2^{-(t+1)} \times 2^m$  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.





**Definition (Round-off error)**

The error resulting from replacing a number with its floating-point form is called *round-off error* or *rounding error*.

**Definition (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**

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

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



## Remark

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

## Definition

In **decimal** expressions, the number  $x^*$  is said to approximate  $x$  to  $t$  **significant digits** if  $t$  is the largest non-negative integer for which

$$\frac{|x - x^*|}{|x|} \leq 5 \times 10^{-t}.$$



- In **binary** expressions, if the floating-point representation  $fl_{\text{chop}}(x)$  for the number  $x$  is obtained by  $t$  digits chopping, then the relative error is

$$\begin{aligned} \frac{|x - fl_{\text{chop}}(x)|}{|x|} &= \frac{|0.00 \cdots 0a_{t+1}a_{t+2} \cdots \times 2^m|}{|1.a_1a_2 \cdots a_t a_{t+1}a_{t+2} \cdots \times 2^m|} \\ &= \frac{|0.a_{t+1}a_{t+2} \cdots|}{|1.a_1a_2 \cdots a_t a_{t+1}a_{t+2} \cdots|} \times 2^{-t}. \end{aligned}$$

The minimal value of the denominator is 1. The numerator is bounded above by 1. As a consequence

$$\left| \frac{x - fl_{\text{chop}}(x)}{x} \right| \leq 2^{-t}.$$



- If  $t$ -digit rounding arithmetic is used and

- $a_{t+1} = 0$ , then  $fl_{\text{round}}(x) = \pm 1.a_1a_2 \cdots a_t \times 2^m$ . A bound for the relative error is

$$\frac{|x - fl_{\text{round}}(x)|}{|x|} = \frac{|0.a_{t+1}a_{t+2} \cdots|}{|1.a_1a_2 \cdots a_t a_{t+1}a_{t+2} \cdots|} \times 2^{-t} \leq 2^{-(t+1)}.$$

The numerator is bounded above by  $\frac{1}{2}$  since  $a_{t+1} = 0$ .

- $a_{t+1} = 1$ , then  $fl_{\text{round}}(x) = \pm(1.a_1a_2 \cdots a_t + 2^{-t}) \times 2^m$ . The upper bound for relative error becomes

$$\frac{|x - fl_{\text{round}}(x)|}{|x|} = \frac{|1 - 0.a_{t+1}a_{t+2} \cdots|}{|1.a_1a_2 \cdots a_t a_{t+1}a_{t+2} \cdots|} \times 2^{-t} \leq 2^{-(t+1)}.$$

The numerator is bounded by  $\frac{1}{2}$  since  $a_{t+1} = 1$ .

Therefore the relative error for rounding arithmetic is

$$\left| \frac{x - fl_{\text{round}}(x)}{x} \right| \leq 2^{-(t+1)} = \frac{1}{2} \times 2^{-t}.$$



## Definition (Machine epsilon)

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

$$fl(x) = x(1 + \delta), \quad |\delta| \leq \varepsilon_M, \quad (1)$$

where  $\varepsilon_M \equiv 2^{-t}$  is referred to as the *machine epsilon*. It is equivalent to the distance from 1.0 to the next largest floating point number, and also equivalent to the least upper bound of relative error resulted from *chopping*.

## Single precision IEEE standard floating-point format

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

$$\varepsilon_M = 2^{-23} \approx 1.192 \times 10^{-7}.$$

This approximately corresponds to **6** accurate decimal digits



## Double precision IEEE standard floating-point format

The mantissa  $f$  corresponds to 52 binary digits (i.e.,  $t = 52$ ), the machine epsilon is

$$\varepsilon_M = 2^{-52} \approx 2.220 \times 10^{-16},$$

which provides between **15** and **16** decimal digits of accuracy. The matlab built-in function `eps` returns this value by default.

## Summary of IEEE standard floating-point format

	single precision	double precision
$\varepsilon_M$	$1.192 \times 10^{-7}$	$2.220 \times 10^{-16}$
smallest positive number	$1.175 \times 10^{-38}$	$2.225 \times 10^{-308}$
largest number	$3.403 \times 10^{38}$	$1.798 \times 10^{308}$
decimal precision	6	15



## Machine Epsilon

- Let  $\odot$  stand for any one of the four basic arithmetic operators  $+$ ,  $-$ ,  $\star$ ,  $\div$ .
- 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

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

where  $\varepsilon_M$  is the machine epsilon. In fact,  $\delta \leq \varepsilon_M/2$  if rounding is used (that is, if  $fl(\cdot) = fl_{\text{round}}(\cdot)$ ).

- But if  $x, y$  are **not** machine numbers, then they must first be rounded to floating-point format before the arithmetic operation. The resulting relative error becomes

$$fl(fl(x) \odot fl(y)) = (x(1 + \delta_1) \odot y(1 + \delta_2))(1 + \delta_3),$$

where  $\delta_i \leq \varepsilon_M, i = 1, 2, 3$ .



# Example

Let  $x = 0.54617$  and  $y = 0.54601$ . With four-digits rounding, we have

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

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

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

$$\frac{|y - y^*|}{|y|} = \frac{0.00001}{0.54601} = 1.8 \times 10^{-5} \leq 5 \times 10^{-5}.$$







## Loss of Significance

- One of the most common error-producing calculations involves the cancellation of significant digits due to the **subtraction of nearly equal numbers**.
- Sometimes, loss of significance can be avoided by rewriting the mathematical formula in equivalent expressions.

## Example

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.



# Solution

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

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

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

$$\frac{|fl(x_1) - x_1|}{|x_1|} = \frac{|-0.02000 + 0.01610723|}{|-0.01610723|} \approx 0.2417 \leq 5 \times 10^{-1}$$



## Loss of Significance

- In calculating  $x_2$ ,

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

and the relative error in computing  $x_2$  is

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

- 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,

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



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  $6.2 \times 10^{-4}$



### Example

Let

$$p(x) = x^3 - 3x^2 + 3x - 1,$$

$$q(x) = ((x - 3)x + 3)x - 1. \quad (\text{nested expression})$$

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



# Solution

With 3-digit rounding for  $p(2.19)$  and  $q(2.19)$ , we have

$$\begin{aligned}
 \hat{p}(2.19) &= ((2.19^3 - 3 \times 2.19^2) + 3 \times 2.19) - 1 \\
 &= ((10.5 - 14.4) + 3 \times 2.19) - 1 \\
 &= (-3.9 + 6.57) - 1 \\
 &= 2.67 - 1 = 1.67 \quad (\text{total } 5 \text{ “} \times \div \text{” and } 3 \text{ “} + - \text{”})
 \end{aligned}$$

and

$$\begin{aligned}
 \hat{q}(2.19) &= ((2.19 - 3) \times 2.19 + 3) \times 2.19 - 1 \\
 &= (-0.81 \times 2.19 + 3) \times 2.19 - 1 \\
 &= (-1.77 + 3) \times 2.19 - 1 \\
 &= 1.23 \times 2.19 - 1 \\
 &= 2.69 - 1 = 1.69 \quad (\text{total } 2 \text{ “} \times \div \text{” and } 3 \text{ “} + - \text{”})
 \end{aligned}$$



With higher precision calculation (more digits), we get

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

Hence the absolute errors are

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

and

$$|q(2.19) - \hat{q}(2.19)| = 0.004841,$$

respectively.

## Conclusion

Nested expression results in less multiplication/division and consequently less accumulation of round-off error.







### Definition (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 (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.

### Remark

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



## Example

Consider the following recurrence algorithm

$$\begin{cases} x_1 = 1, & x_2 = \frac{1}{3} \\ x_n = \frac{13}{3}x_{n-1} - \frac{4}{3}x_{n-2} \end{cases}$$

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

A Matlab implementation of the recurrence algorithm is as follows:



## 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);
    xstar = (1/3)^(ii-1);
    RelErr = abs(xstar-x(ii)) / xstar;
    fprintf('x(%2.0f) = %20.8d, x_ast(%2.0f) = %20.8d,
        RelErr(%2.0f) = %14.4d \n', ...
        ii,x(ii),ii,xstar,ii,RelErr);
end
```



Result of the Matlab implementation:

$n$	$x_n^h$ (numerical)	$x_n^e$ (exact)	RelErr
9	4.57247371e-04	4.57247371e-04	4.4359e-10
11	5.08052602e-05	5.08052634e-05	6.3878e-08
13	5.64497734e-06	5.64502927e-06	9.1984e-06
15	6.26394672e-07	6.27225474e-07	1.3246e-03
16	2.05751947e-07	2.09075158e-07	1.5895e-02
17	5.63988754e-08	6.96917194e-08	1.9074e-01
18	-2.99408028e-08	2.32305731e-08	2.2889e+00

The relative error is increased by a factor of 12 after each iteration (compare the result from  $n = 9$  to  $n = 11$  and from  $n = 16$  to  $n = 17$ , etc). This is a typical example of **exponential instability**, where the error grows exponentially in  $n$ .



**Question:** What is the source of this instability and where does the factor 12 come from?

### Proposition

The general solution of the three term recursion formula

$x_{n+1} = ax_n + bx_{n-1}$  is given by

$$x_n = c_1 z_1^n + c_2 z_2^n \quad (3)$$

where  $z_1$  and  $z_2$  are the (distinct) roots of the characteristic equation  $z^2 = az + b$ . In case  $z_1 = z_2$ , equation (3) is replaced by  $x_n = c_1 z_1^n + c_2 n z_1^n$ .

In this example,  $z_1 = 1/3$  and  $z_2 = 4$ . The fact that  $|z_2| > |z_1|$  is precisely the reason for exponential instability.



Denote by  $x_n^e$  the exact solution and  $x_n^h$  the numerical solution. We have

$$\begin{cases} x_1^e = 1, & x_2^e = \frac{1}{3} \\ x_n^e = \frac{13}{3}x_{n-1}^e - \frac{4}{3}x_{n-2}^e \end{cases}$$

and

$$\begin{cases} x_1^h = fl(1) = 1, & x_2^h = fl(\frac{1}{3}) = \frac{1}{3}(1 + \delta_2) \\ x_n^h = (\frac{13}{3}(1 + \alpha_n)x_{n-1}^h - \frac{4}{3}(1 + \beta_n)x_{n-2}^h) (1 + \delta_n) \end{cases}$$

where  $|\delta_n|, |\alpha_n|, |\beta_n| \leq \varepsilon_M$ . Loosely speaking, the behavior of  $x_n^h$  can be approximated by  $x_n^h = \frac{13}{3}x_{n-1}^h - \frac{4}{3}x_{n-2}^h$ , thus the error  $e_n := x_n^h - x_n^e$  satisfies (approximately)  $e_n = \frac{13}{3}e_{n-1} - \frac{4}{3}e_{n-2}$ . The general solution is given by  $e_n = d_1(\frac{1}{3})^n + d_24^n$ . Since  $e_1 = 0$  and  $e_2 = \frac{1}{3}\delta_1 \neq 0$ , it follows that  $d_2 \neq 0$  and the error grows exponentially in  $n$ .

The above argument is not completely rigorous, but is the essential part of the error estimate and can be made rigorous with some elaboration.



## Definition

Suppose  $\{\beta_n\} \rightarrow 0$  and  $\{x_n\} \rightarrow x^*$ . 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

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

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



# Solution:

Note that both

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

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

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

Hence

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

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

