Numerical Analysis / Numerical Methods

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Lecture 1 (part 3), Spring 2022

Significant digits

Let x_T and x_A be true and, respectively approximated values.

Definition

We say that approximation x_A has m **significant digits** with respect to true value x_T if $|err(x_A)| \leqslant 5$ units in the $(m+1)$-st digit, beginning with the first nonzero digit in x_T.

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Example

Let

$$
\begin{aligned}
x_T &= e = 2.71828182845904523\ldots, \\
x_A &= \frac{19}{7} = 2.71428571428571428 5\ldots, \\
err(x_A) &\approx 0.003996\ldots
\end{aligned}
$$

Therefore, there are 3 significant digits in this approximation.

Significant digits

Another way to look at significant digits (also called significant figures) regardless whether we have an approximation or not is each of the digits of a number that are used to express it to the required degree of accuracy, starting from the first non-zero digit.

There are several rules:

- All non-zero numbers are significant.
  The number 37.9 has 3 significant digits.
- Zeros between two non-zero digits are significant.
  The number 4001.7 has 5 significant digits,
  while the number 2005 has 4 significant digits.
- Leading zeros are not significant.
  The number 0.89 has only 2 significant digits, and 0.00017 also has 2 significant digits.
- Trailing zeros to the right of the decimal are significant.
  There are 4 significant digits in 92.00 and 5 significant digits in 3.0000.

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and consider evaluating it on a 6-digit decimal calculator which uses rounded arithmetic.

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x	Computed $f(x)$	True $f(x)$	Error
1	0.4142210	0.414214	$7.0000e-006$
10	1.54340	1.54347	$-7.0000e-005$
100	4.99000	4.98756	0.0024
1000	15.8000	15.8074	-0.0074
10000	50.0000	49.9988	0.0012
100000	100.000	158.113	-58.1130

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Three significant digits in $\sqrt{x+1} = \sqrt{101}$ have been lost from $\sqrt{x} = \sqrt{100}$.

The loss of precision is due to the form of the function $f(x)$ and the finiteness of the precision of the 6 digit calculator.

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In this particular case, we can avoid the loss of precision by rewriting the function as follows:

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$$\begin{aligned} f(x) &= x\frac{\sqrt{x+1}+\sqrt{x}}{\sqrt{x+1}+\sqrt{x}} \cdot \frac{\sqrt{x+1}-\sqrt{x}}{1} \\ &= \frac{x}{\sqrt{x+1}+\sqrt{x}}. \end{aligned}$$

Thus we will avoid the subtraction on near quantities.

Doing so gives us

$$f(100) = 4.98756,$$

a value with 6 significant digits.

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x	Computed $f(x)$	True $f(x)$	Error
0.1	0.4995834700	0.4995834722	$-2.2000e-009$
0.01	0.4999960000	0.4999958333	$1.6670e-007$
0.001	0.5000000000	0.4999999583	$4.1700e-008$
0.0001	0.5000000000	0.4999999996	$4.0000e-010$
0.00001	0.0	0.5000000000	0.5

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Then on the calculator:

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\begin{aligned}
\cos(0.001) &= 0.9999994999 \\
1 - \cos(0.001) &= 5.001 \times 10^{-7} \\
\frac{1 - \cos(0.001)}{(0.001)^2} &= 0.5001000000
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There are 3 significant digits in the answer.

How can such a straightforward and short calculation lead to such a large error (relative to the accuracy of the calculator)?

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The last example, fortunately, can be fixed in a number of ways. Easiest is to use a trigonometric identity:

$$\cos(x) = 1 - 2\sin^2(x/2),$$

$$f(x) = \frac{1-\cos x}{x^2} = \frac{2\sin^2(x/2)}{x^2} = \frac{1}{2}\left(\frac{\sin(x/2)}{x/2}\right)^2.$$

This latter formula, with $x = 0.001$, yields a computed value of 0.4999999584, nearly the true answer. We could also have used a Taylor polynomial for $\cos(x)$ around $x = 0$ to obtain a better approximation to $f(x)$ for small values of x.

Example 3. Evaluate e^{-5} using a Taylor polynomial approximation:

$$e^{-5} = 1 + \frac{(-5)}{1!} + \frac{(-5)^2}{2!} + \frac{(-5)^3}{3!} + \frac{(-5)^4}{4!} + \frac{(-5)^5}{5!} + \frac{(-5)^6}{6!} \dots$$

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To make the point about cancellation more strongly, imagine that each of the terms in the above polynomial is calculated exactly and then rounded to the arithmetic of the computer. We add the terms exactly and then we round to four digits.

Loss of significance errors. Example 3

Degree	Term	Sum	Degree	Term	Sum
0	1.000	1.000	13	-0.1960	-0.04230
1	-5.000	-4.000	14	$0.7001e-1$	0.02771
2	12.50	8.500	15	$-0.2334e-1$	0.004370
3	-20.83	-12.33	16	$0.7293e-2$	0.01166
4	26.04	13.71	17	$-0.2145e-2$	0.009518
5	-26.04	-12.33	18	$0.5958e-3$	0.01011
6	21.70	9.370	19	$-0.1568e-3$	0.009957
7	-15.50	-6.130	20	$0.3920e-4$	0.009996
8	9.688	3.558	21	$-0.9333e-5$	0.009987
9	-5.382	-1.824	22	$0.2121e-5$	0.009989
10	2.691	0.8670	23	$-0.4611e-6$	0.009989
11	-1.223	-0.3560	24	$0.9670e-7$	0.009989
12	0.5097	0.1537	25	$-0.1921e-7$	0.009989

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12	0.5097	0.1537	25	$-0.1921e-7$	0.009989

True answer is 0.006738!

Loss of significance errors. Example 3

Look at the numbers being added and their accuracy, ex. 3rd term:

$$\frac{(-5)^3}{3!} = -\frac{125}{6} = -20.83$$

in the 4 digit decimal calculation, with an error of magnitude 0.00333.

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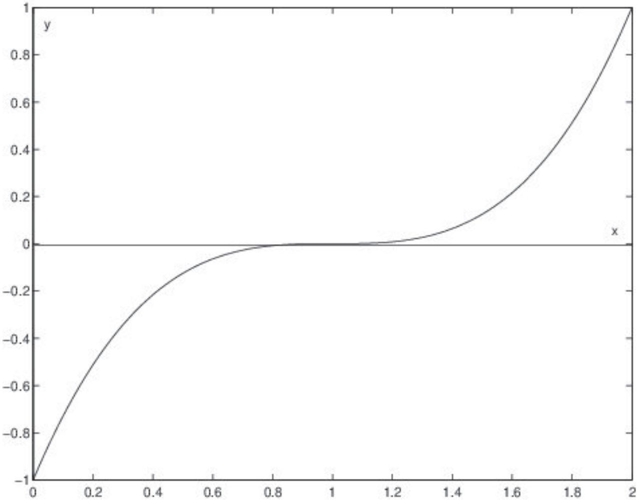
General principle

Whenever a sum is being formed in which the final answer is much smaller than some of the terms being combined, then a loss of significance error is occurring.

Noise in function evaluation

Consider plotting the function

$$f(x) = (x-1)^3 = x^3 - 3x^2 + 3x - 1 = -1 + x(3 + x(-3 + x)).$$



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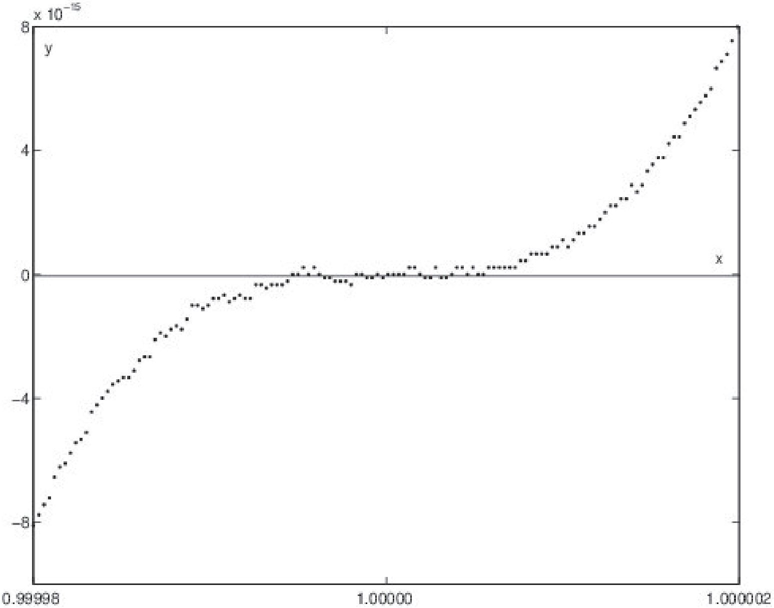

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This noise is generally "random" and small.

But it can affect the accuracy of other calculations which depend on $f(x)$.

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Thus, $f(x)$ will be stored as zero if

$$\begin{aligned} x^{10} &< m, \\ |x| &< m^{\frac{1}{10}}, \\ |x| &< 1.61 \times 10^{-4}, \\ -0.000161 < x &< 0.000161. \end{aligned}$$

Storing a nonzero number as a zero leads to **underflow error**.

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$$m = 2^{128}\left(1 - 2^{-24}\right) = 3.40 \times 10^{38}$$

Thus, $f(x)$ will overflow if

$$\begin{aligned} x^{10} &> m, \\ |x| &> m^{\frac{1}{10}}, \\ |x| &> 7131.6 \end{aligned}$$

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The error in $x_A \, \omega^* \, y_A$ can be rewritten as:

$$x_T \, \omega \, y_T - x_A \, \omega^* \, y_A = \left[x_T \, \omega \, y_T - x_A \, \omega \, y_A\right] + \left[x_A \, \omega \, y_A - x_A \, \omega^* \, y_A\right]$$

The last term is the error introduced by the inexactness of the machine arithmetic, since it can be shown that

$$\mathrm{Rel}(x_A \, \omega^* \, y_A) = -\varepsilon.$$

With rounded binary arithmetic having n digits in the mantissa,

$$-2^{-n} \leq \varepsilon \leq 2^{-n}.$$

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Coming back to error formula we have

$$x_T\,\omega\,y_T - x_A\,\omega^*\,y_A = \left[x_T\,\omega\,y_T - x_A\,\omega\,y_A\right] + \underbrace{\left[x_A\,\omega\,y_A - x_A\,\omega^*\,y_A\right]}_{\text{Relative error is } -\varepsilon}.$$

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The first term from the right side

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Let $\omega = *$ (i.e. multiplication). Write

$$x_T = x_A + \xi, \qquad y_T = y_A + \eta,$$

where ξ and η are the approximation errors is x_A and y_A.

Propagation of arithmetic operations errors

Then for the relative error in $x_A\, y_A$

$$\begin{aligned}
\mathrm{Rel}(x_A * y_A) &= \frac{x_T * y_T - x_A * y_A}{x_T * y_T} \\
&= \frac{x_T * y_T - (x_T - \xi) * (y_T - \eta)}{x_T * y_T} \\
&= \frac{x_T \eta + y_T \xi - \xi \eta}{x_T * y_T} \\
&= \frac{\xi}{x_T} + \frac{\eta}{y_T} - \frac{\xi}{x_T} \cdot \frac{\eta}{y_T} \\
&= \mathrm{Rel}(x_A) + \mathrm{Rel}(y_A) - \mathrm{Rel}(x_A) \cdot \mathrm{Rel}(y_A).
\end{aligned}$$

Then for the relative error in $x_A\, y_A$

$$\begin{aligned}
\mathrm{Rel}(x_A * y_A) &= \frac{x_T * y_T - x_A * y_A}{x_T * y_T} \\
&= \frac{x_T * y_T - (x_T - \xi) * (y_T - \eta)}{x_T * y_T} \\
&= \frac{x_T\eta + y_T\xi - \xi\eta}{x_T * y_T} \\
&= \frac{\xi}{x_T} + \frac{\eta}{y_T} - \frac{\xi}{x_T} \cdot \frac{\eta}{y_T} \\
&= \mathrm{Rel}(x_A) + \mathrm{Rel}(y_A) - \mathrm{Rel}(x_A) \cdot \mathrm{Rel}(y_A).
\end{aligned}$$

Usually we have $|\mathrm{Rel}(x_A)| \ll 1, \quad |\mathrm{Rel}(y_A)| \ll 1$. Therefore, we can skip the last term $\mathrm{Rel}(x_A) \cdot \mathrm{Rel}(\, y_A)$, since it is much smaller compared with previous two.

$$\begin{aligned}
\mathrm{Rel}(x_A y_A) &= Rel(x_A) + Rel(y_A) - \mathrm{Rel}(x_A) \cdot \mathrm{Rel}(y_A) \\
&\approx \mathrm{Rel}(x_A) + \mathrm{Rel}(y_A).
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However, there is a more subtle error occurring here.

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We want to calculate $f(x_T)$, but instead we evaluate $\widetilde{f}(x_A)$.

What can we say about the error in this latter computed quantity?

Rewrite the error

$$f(x_T) - \widetilde{f}(x_A) = \left[f(x_T) - f(x_A)\right] + \left[f(x_A) - \widetilde{f}(x_A)\right].$$

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The quantity $f(x_T) - f(x_A)$ is called the **propagated error**. It is the error that results from using perfect arithmetic in the evaluation of the function.

If the function $f(x)$ is differentiable, then we can use the **Mean-value Theorem** from calculus to write

$$f(x_T) - f(x_A) = f'(\xi)(x_T - x_A)$$

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Since usually x_T and x_A are close together, we can say ξ is close to either of them, and

$$\begin{aligned} f(x_T) - f(x_A) &= f'(\xi)(x_T - x_A) \\ &\approx f'(x_T)(x_T - x_A) \\ &\approx f'(x_A)(x_T - x_A). \end{aligned}$$

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This last approximation can be used in practice to estimate the propagated error once function f and its derivative are known.

Example. Define $f(x) = b^x$, where b is a positive real number. Then, last formula yields

$$b^{x_T} - b^{x_A} \approx (\ln b) b^{x_T} (x_T - x_A).$$

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Therefore,

$$\begin{aligned} \operatorname{Rel}\left(b^{x_A}\right) &\approx \frac{(\ln b) b^{x_T} (x_T - x_A)}{b^{x_T}} \\ &= \frac{(\ln b)(x_T - x_A) x_T}{x_T} \\ &= x_T \ln b \cdot \operatorname{Rel}(x_A) \\ &= K \cdot \operatorname{Rel}(x_A). \end{aligned}$$

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The number K is called a **condition number** for the computation.

Summation

Let S be a sum with a relatively large number of terms

$$S = a_1 + a_2 + \ldots a_n, \tag{1}$$

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Define

$$\begin{aligned}
S_2 &= fl(a_1 + a_2),\\
S_3 &= fl(S_2 + a_3),\\
S_4 &= fl(S_3 + a_4),\\
&\vdots\\
S_n &= fl(S_{n-1} + a_n).
\end{aligned}$$

Recall the formula

$$fl(x) = x(1+\varepsilon).$$

Summation

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S_2 &= (a_1 + a_2)(1 + \varepsilon_2), \\
S_3 &= (S_2 + a_3)(1 + \varepsilon_3), \\
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\begin{aligned}
S_3 &= (S_2 + a_3)(1 + \varepsilon_3), \\
&= ((a_1 + a_2)(1 + \varepsilon_2) + a_3)(1 + \varepsilon_3), \\
&\approx (a_1 + a_2 + a_3) + a_1(\varepsilon_2 + \varepsilon_3), \\
&+ a_2(\varepsilon_2 + \varepsilon_3) + a_3\varepsilon_3, \\
S_4 &\approx (a_1 + a_2 + a_3 + a_4) + a_1(\varepsilon_2 + \varepsilon_3 + \varepsilon_4) \\
&+ a_2(\varepsilon_2 + \varepsilon_3 + \varepsilon_4) + a_3(\varepsilon_3 + \varepsilon_4) + a_4\varepsilon_4.
\end{aligned}
$$

And finally we get

$$\begin{aligned} S_n \approx (a_1 + a_2 + \ldots + a_n) &+ a_1(\varepsilon_2 + \ldots + \varepsilon_n) \\ + a_2(\varepsilon_2 + \ldots + \varepsilon_n) &+ a_3(\varepsilon_3 + \ldots + \varepsilon_n) \\ + a_4(\varepsilon_4 + \ldots + \varepsilon_n) &+ \ldots + a_n\varepsilon_n. \end{aligned}$$

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We are interested in the error $S - S_n$:

$$\begin{aligned} S - S_n \approx\, &-a_1(\varepsilon_2 + \ldots + \varepsilon_n) - a_2(\varepsilon_2 + \ldots + \varepsilon_n) - a_3(\varepsilon_3 + \ldots + \varepsilon_n) \\ &- a_4(\varepsilon_4 + \ldots + \varepsilon_n) - \ldots - a_n\varepsilon_n. \end{aligned}$$

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Using the last relation, in order to minimize the error $S - S_n$, we can establish the strategy for summation:
initially rearrange the terms in increasing order:

$$|a_1| \leq |a_2| \leq |a_3| \leq \ldots \leq |a_n|.$$

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$$\begin{aligned} S_n \approx (a_1 + a_2 + \ldots + a_n) + a_1(\varepsilon_2 + \ldots + \varepsilon_n) \\ + a_2(\varepsilon_2 + \ldots + \varepsilon_n) + a_3(\varepsilon_3 + \ldots + \varepsilon_n) \\ + a_4(\varepsilon_4 + \ldots + \varepsilon_n) + \ldots + a_n\varepsilon_n. \end{aligned}$$

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In this rearrangement, smaller numbers a_1 and a_2 will be multiplied with larger numbers $\varepsilon_2 + \ldots + \varepsilon_n$, and a larger number a_n will be multiplied with a smaller number ε_n.

Summation. Example with chopping

Four digit calculator with chopping is being used to compute the following sum:

$$S = \sum_{i=1}^{n} \frac{1}{i} = 1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{n}.$$

Number of terms, n	Exact value	SL	Error	LS	Error
10	2.929	2.928	0.001	2.927	0.002
25	3.816	3.813	0.003	3.806	0.010
50	4.499	4.491	0.008	4.470	0.020
100	5.187	5.170	0.017	5.142	0.045
200	5.878	5.841	0.037	5.786	0.092
500	6.793	6.692	0.101	6.569	0.224
1000	7.486	7.284	0.202	7.069	0.417

SL: *smallest to largest* strategy; LS: *largest to smallest* strategy.

Summation. Example with rounding

Four digit calculator with rounding is being used to compute the following sum:

$$S = \sum_{i=1}^{n} \frac{1}{i} = 1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{n}.$$

Number of terms, n	Exact value	SL	Error	LS	Error
10	2.929	2.929	0	2.929	0
25	3.816	3.816	0	3.817	-0.001
50	4.499	4.500	-0.001	4.498	0.001
100	5.187	5.187	0	5.187	0
200	5.878	5.878	0	5.876	0.002
500	6.793	6.794	-0.001	6.783	0.010
1000	7.486	7.486	0	7.449	0.037

SL: *smallest-to-largest* strategy; LS: *largest-to-smallest* strategy.

Conclusions:

1. *Smallest-to-largest* strategy is more preferable than the *largest-to-smallest*, since the error in the first strategy is at least twice as small.

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Conclusions:

1. *Smallest-to-largest* strategy is more preferable than the *largest-to-smallest*, since the error in the first strategy is at least twice as small.
2. Rounding is much better that chopping. Just compare the errors in the first and second tables.
3. Observe that in the rounding case, some of the errors are 0, since rounding errors can be either positive or negative, and thus they might cancel each other.