$\begin{array}{c} {\rm Numerical~Analysis} \\ {\it Theory} \end{array}$

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Chapter 1

Introduction

1.1 Numerical analysis and errors

Numerical analysis is the field of mathematics dealing with methods to find the solutions of certain mathematical problems with an electronic calculator. It is the intersection between math and computer science.

On the other hand, scientific computing also deals with the model formalization and so it needs also engineering knowledge.

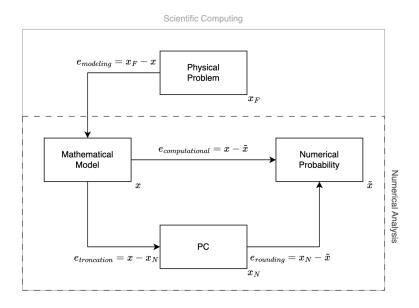


Figure 1.1: Difference between numerical analysis and scientific computing

As it is possible to see from the diagram every step of the computation have to deal with errors. The possible types of errors are:

• Absolute: $|x - \tilde{x}|$

• Relative: $\frac{|x-\tilde{x}|}{|x|}$, where $x \neq 0$

The relative error is more precise because it compares the error with the measure quantity.

Example: Let us consider x = 100 and $\tilde{x} = 100.1$. The errors in this case are:

$$e_{abs} = |x - \tilde{x}| = |100 - 100.1| = 0.1$$

$$e_{rel} = \frac{|x - \tilde{x}|}{|x|} = \frac{|100 - 100.1|}{|100|} = 0.001$$

Let us consider x = 0.2 and $\tilde{x} = 0.1$. The errors in this case are:

$$e_{abs} = |x - \tilde{x}| = |0.2 - 0.1| = 0.1$$

$$e_{rel} = \frac{|x - \tilde{x}|}{|x|} = \frac{|0.2 - 0.1|}{|0.2|} = 0.5$$

The result are that the measures have the same absolute error (10%), but the relative error is much grater in the second example (50% vs 0.1%). This result proves that the relative error is the most precise.

1.2 Floating point

A calculator can only handle a finite quantity of numbers and compute a finite number of operations. For those reason the set of the real numbers \mathbb{R} is indeed represented by a finite set of machine numbers $\mathbb{F} = \{-\tilde{a}_{min}, \dots, \tilde{a}_{max}\}$ called floating points numbers. The function used to find the corresponding value in \mathbb{F} to a number in \mathbb{R} is fl(x) that does an operation called truncation and rounding.

The set $\mathbb{F} = \mathbb{F}(\beta, t, L, U)$ is characterized by four parameters β, t, L and U such that every real number $fl(x) \in \mathbb{F}$ can be written as:

$$fl(x) = (-1)^s m \beta^{e-t} = (-1)^s (a_1 a_2 \dots a_t)_\beta \beta^{e-t}$$

where:

- $\beta \geq 2$ is the basics, an integer that determines the numeric system.
- $m = (a_1 a_2 \dots a_t)_{\beta}$ is the mantissa, $(0 < m < \beta^t 1)$ where t is the number of digits such that $0 < a_1 \le \beta 1$ and $0 \le a_i \le \beta 1$ for $i = 2, \dots, t$.

- $e = \mathbb{Z}$ is the exponent such that L < e < U, with L < 0 and U > 0.
- $s = \{0, 1\}$ is the sign.

In the definition of the numbers in the mantissa set we have to set the constraint $a_1 \neq 0$ to ensure the uniqueness of the representation.

The set of floating points has the following characteristic values:

• Machine epsilon, that is the distance between one and the smallest floating point number greater than one, and it is equal to:

$$\epsilon_M = \beta^{1-t}$$

• Round-off error, that is the relative error that is committed when substituting $x \in \mathbb{R} - \{0\}$ with his corresponding $fl(x) \in \mathbb{F}$. It is limited by:

$$\frac{|x - fl(x)|}{|x|} \le \frac{1}{2} \epsilon_M$$

where $x \neq 0$.

• Cardinality of the floating point set:

$$\#\mathbb{F} = 2\beta^{t-1}(\beta - 1)(U - L + 1) + 1$$

where:

- -2 is needed to consider both positive and negative numbers.
- $-\beta^{t-1}$ is the cardinality of values that can be taken by all digits.
- $-(\beta-1)$ is the cardinality of values that can be taken by a_1 .
- -(U-L+1) considers all the possible variations for the exponent.
- 1 is needed to consider also the zero.
- The biggest and the smallest numbers in the set are found with the formula:

$$x_{min} = \beta^{L-1}$$
$$x_{max} = \beta^{U} (1 - \beta^{-t})$$

Example: In MATHLAB the floating point set is defined with the following variables:

$$(\beta = 2, t = 53, L = -1021, U = 1024)$$

With the command *eps* we can find the machine epsilon, that in MATLAB case is:

$$\epsilon_M = 2.22 \cdot 10^{-16}$$

With the command realmin and realmax we can find the smallest and the largest numbers representable that are equal to:

$$x_{min} = 2.225073858507201 \cdot 10^{-308}$$

$$x_{max} = 1.797693134862316 \cdot 10^{308}$$

Since not all the numbers in the \mathbb{R} set are also in the \mathbb{F} set, in the second one there is no continuity. It is possible to demonstrate that while we are increasing the values of the numbers we are also increasing the distance between two consecutive numbers in \mathbb{F} .

Example: Let us consider the floating number set $\mathbb{F}(2,2,-1,2)$. The characteristic values of this set are:

- $\epsilon_M = \beta^{1-t} = 0.5$.
- $x_{min} = \beta^{L-1} = 0.25$.
- $x_{max} = \beta^U (1 \beta^t) = 3.$
- $\#\mathbb{F} = 2\beta^{t-1}(\beta 1)(U L + 1) + 1 = 16.$

The exponent can have the values -1, 0, 1 and 2. The mantissa will be like $(a_1a_2)_{\beta}$ because t=2. The possible positive values are reported in the figure.

The other important aspect is that the passage between the two sets causes the loss of two important properties such as associativity end the neutral number for the sum.

Chapter 2

Nonlinear equations

2.1 Iterative methods

To solve a nonlinear equation f we have to find $\alpha \in \mathbb{R}$ that is a zero of f such that $f(\alpha) = 0$. The set of all the polynomials of degree n is denoted by the symbol \mathbb{P}_n that contains all the polynomial that have a grade less or equal to n.

Theorem $(Abel-Ruffini\ theorem)$

There is no solution in radicals to general polynomial equations of degree five or higher with arbitrary coefficients.

So, to solve polynomials with a degree higher than four we need to use the iterative methods. The general idea of those methods is the following:

- 1. Select an arbitrary initial value $x^{(0)}$ called initial guess, that is a hypothetical value for α .
- 2. Use the selected value as an input for a black-box function.
- 3. Use the output of the black-box function as the new $x^{(0)}$ and return to point one.

After some iterations (that depends on the chosen method) we will have a set of values $\{x^{(n)}\}$ convergent such that:

$$\lim_{n\to\infty} = \alpha$$

and the error related to the value found for α is equal to:

$$\lim_{n \to \infty} e^n = 0$$

That implies that the error can be also written as:

$$e^n = \alpha - x^{(n)}$$

2.2 Bisection method

Theorem (Theorem of zeros of continuous functions)

Let f(x) be a continuous function on the interval I=(a,b), that is $f\in C^0([a,b])$. If f(a)f(b)<0, then there exists at least one zero $\alpha\in I$ of f(x).

Let us assume that exist a unique zero, and let us call it α .

The strategy of the bisection method is to have the given interval and select a sub-interval where f features a sign change. Following such procedure it is guaranteed that every interval selected this way will contain α . The sequence $\{x^{(k)}\}$ of the midpoints of these sub-intervals will inevitably tend to α since the length of the sub-intervals tends to zero as k tends to infinity.

Algorithm 1 Algorithm for the bisection method

```
1: a^{(0)} \leftarrow a, b^{(0)} \leftarrow b, x^{(0)} \leftarrow \overline{a^{(0)} + b^{(0)}}
 2: while stopping criterion not satisfied do
           if f(x^{(k+1)}) = 0 then
 3:
                 \alpha \leftarrow x^{(k+1)}
 4:
                 return
 5:
 6:
           else
                if f(x^{(k-1)})f(a^{(k-1)}) < 0 then
 7:
                      a^{(k)} \leftarrow a^{(k-1)}
 8:
                      b^{(k)} \leftarrow x^{(k-1)}
 9:
                 end if
10:
                 if f(x^{(k-1)})f(b^{(k-1)}) < 0 then
11:
                      a^{(k)} \leftarrow x^{(k-1)}
12:
                      b^{(k)} \leftarrow b^{(k-1)}
13:
                end if x^{(k)} \leftarrow \frac{a^{(k)} + b^{(k)}}{2}
14:
15:
16:
           end if
17: end while
18: return
```

The dimension of the k interval is given from the formula:

$$\left|I^{(k)}\right| = \frac{b-a}{2^k}$$

where k > 0. We said that the error is equal to $e^{(k)} := |x^{(k)} - \alpha|$. So, it is also possible to estimate the error with an upper bound, that is an error

estimator. We have that.

$$e^{(k)} = |x^{(k)} - \alpha| < \frac{1}{2} |I^{(k)}| = (b - a) \left(\frac{1}{2}\right)^{(k+1)}$$

This result implies that this method is convergent, in fact the error is monotonic descending.

Given the tolerance TOL > 0 it is possible to calculate the minimum number of iterations of the bisection method, defined as k_{min} , such that $e^{(k_{min})} < TOL$. In fact, from the previous equation we obtain that:

$$k_{min} > \log_2\left(\frac{b-a}{TOL}\right) - 1$$

STOPPING criterion

2.3 Newton method

2.4 Fixed-point method

Chapter 3 Linear equations