

Numerical Analysis
Theory

Christian Rossi

Academic Year 2023-2024

Abstract

The topics of the course are:

- Floating-point arithmetic: different sources of the computational error; absolute vs relative errors; the floating point representation of real numbers; the round-off unit; the machine epsilon; floating-point operations; over- and under-flow; numerical cancellation.
- Numerical approximation of nonlinear equations: the bisection and the Newton methods; the fixed-point iteration; convergence analysis (global and local results); order of convergence; stopping criteria and corresponding reliability; generalization to the system of nonlinear equations (hints).
- Numerical approximation of systems of linear equations: direct methods (Gaussian elimination method; LU and Cholesky factorizations; pivoting; sparse systems: Thomas algorithm for tridiagonal systems); iterative methods (the stationary and the dynamic Richardson scheme; Jacobi, Gauss-Seidel, gradient, conjugate gradient methods (hints); choice of the preconditioner; stopping criteria and corresponding reliability); accuracy and stability of the approximation; the condition number of a matrix; over- and under-determined systems: the singular value decomposition (hints).
- Numerical approximation of functions and data: Polynomial interpolation (Lagrange form); piecewise interpolation; cubic interpolating splines; least-squares approximation of clouds of data.
- Numerical approximation of derivatives: finite difference schemes of the first and second order; the undetermined coefficient method.
- Numerical approximation of definite integrals: simple and composite formulas; midpoint, trapezoidal, Cavalieri-Simpson quadrature rules; Gaussian formulas; degree of exactness and order of accuracy of a quadrature rule.
- Numerical approximation of ODEs: the Cauchy problem; one-step methods (forward and backward Euler and Crank-Nicolson schemes); consistency, stability, and convergence (hints).

Contents

1	Introduction	2
1.1	Numerical analysis and errors	2
1.2	Floating point	3
2	Nonlinear equations	6
2.1	Introduction	6
2.2	Iterative methods	6
2.3	Stopping conditions	7
2.4	Bisection method	8
2.5	Newton method	9
2.6	Secant method	11
2.7	Systems of nonlinear equations	11
2.8	Fixed point method	11

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.

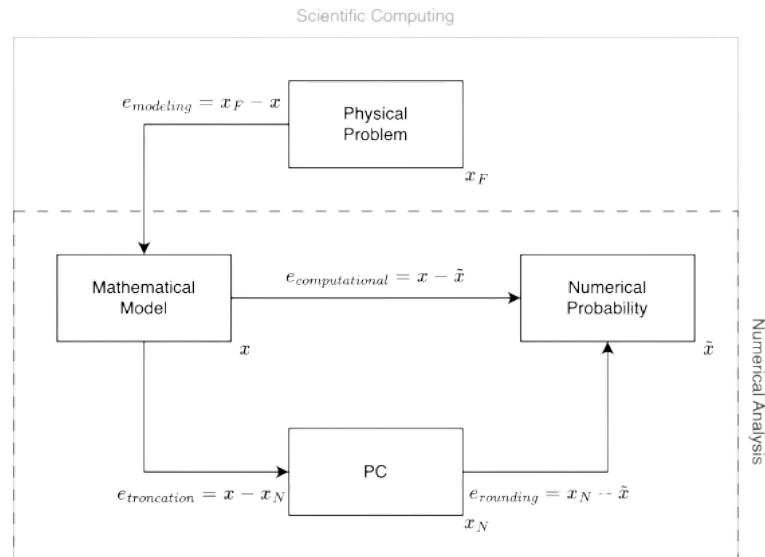


Figure 1.1: Difference between numerical analysis and scientific computing

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:

$$fl(x) = (-1)^s (0.a_1 a_2 \dots a_t) \beta^e$$

where:

- $\beta \geq 2$ is the basics, an integer that determines the numeric system.
- $m = (0.a_1 a_2 \dots a_t)$ is the mantissa.
- $e \in \mathbb{Z}$ 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. In this case we say that the number is normalized.

The set of floating points has the following characteristic values are:

- 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:

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

where $x \neq 0$.

- The biggest and the smallest numbers in the set are found with the formula:

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

Example : In MATLAB 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:

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

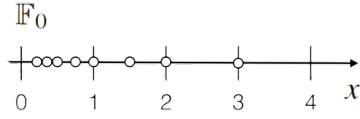
$$x_{max} = 1.797693134862316 \cdot 10^{308}$$

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.



e	-1	0	1	2
$m = (10)_2 = 2$	$\frac{1}{4}$	$\frac{1}{2}$	1	2
$m = (11)_2 = 3$	$\frac{3}{8}$	$\frac{3}{4}$	$\frac{3}{2}$	3

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

Chapter 2

Nonlinear equations

2.1 Introduction

To solve a nonlinear equation $f(x)$ we have to find $\alpha \in \mathbb{R}$ that is a zero of f such that $f(\alpha) = 0$.

Definition

The point α is said to be a *zero with multiplicity m* if:

- $f(\alpha) = f'(\alpha) = \dots = f^{(m-1)}(\alpha) = 0$.
- $f^{(m)}(\alpha) \neq 0$.

If m is odd the function changes sign across the zero. It does not change the sign if n is even.

2.2 Iterative methods

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:

$$\lim_{n \rightarrow \infty} x^{(n)} = \alpha$$

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

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

That implies that the error can be also written as:

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

All the methods we are going to see constructs a sequence $x^{(1)}, x^{(2)}, \dots, x^{(n)}$ of numbers that hopefully converges to α :

$$\lim_{k \rightarrow +\infty} |x^{(k)} - \alpha| = 0$$

Definition (*order of convergence*)

An iterative method for the approximation of the zero α of the function $f(x)$ is convergent with order q if and only if for $k > k_0$:

$$|x^{(k)} - \alpha| \leq c |x^{(k+1)} - \alpha|^q$$

We can have two cases:

- If $q = 1$ it is called linear convergence and there are the constraint $0 < c < 1$.
- If $q > 1$, c can be any positive number greater than zero.

2.3 Stopping conditions

The iterative methods needs a stopping criterion. It can be on four possible conditions:

- On the error, stops if $|x^{(k)} - \alpha| \leq \epsilon_e$.

- On the residual, stops if $|f(x^{(k)})| \leq \epsilon_r$.
- On the step length, stops if $|x^{(k)} - x^{(k-1)}| \leq \epsilon_s$.
- On the max numbers of iterations, stops if $k \leq k_{max}$.

If none of the first three stopping criterions are satisfied, it means that there are no convergence.

2.4 Bisection method

Theorem (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. We have that:

$$|x^{(k)} - \alpha| \leq \frac{1}{2} |b^{(k)} - a^{(k)}|$$

So, since the first part of the equation is similar to the condition on the error, we have that the stopping criterion will be:

$$|b^{(k)} - a^{(k)}| \leq 2\epsilon_e$$

Now that we have the tolerance ϵ we can find that:

$$k_{min} = \left\lceil \log_2 \left(\frac{|b - a|}{\epsilon} \right) - 1 \right\rceil$$

The inputs for the algorithm are: a function $f \in C(\mathbb{R})$ and an interval $[a, b]$ such that $f(a)f(b) \leq 0$.

Algorithm 1 Algorithm for the bisection method

```
1: for  $k = 0, 1, \dots, n$  do
2:    $x^{(k)} = \frac{a + b}{2}$ 
3:   if  $|b^{(k)} - a^{(k)}| \leq 2\epsilon_e$  then
4:     return  $x^{(k)}$ 
5:   else if  $f(x^{(k)})f(a) < 0$  then
6:      $b \leftarrow x^{(k)}$ 
7:   else
8:      $a \leftarrow x^{(k)}$ 
9:   end if
10: end for
```

The pros are:

- I can control the maximal error.
- Convergence is guaranteed.
- Use only evaluation of f

The cons are:

- Work only if f changes sign.
- Convergence is slow.

2.5 Newton method

The sign of the given function f at the endpoints of the sub-intervals is the only information exploited by the bisection method. A more efficient method can be constructed by exploiting the values attained by f and its derivative. If f is differentiable we have that:

$$y(x) = f(x^{(k)}) + f'(x^{(k)})(x - x^{(k)})$$

provides the equation of the tangent to the curve $(x, f(x))$ at the point $x^{(k)}$. If we pretend that $x^{(k+1)}$ is such that $f(x^{(k+1)}) = 0$, we obtain:

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})} \quad k \geq 0$$

provided $f'(x^{(k)}) \neq 0$. This method is known as Newton's method and corresponds to computing the zero of f locally replacing f by its tangent line.

Obviously, this method converges in a single step when f is linear.

The Newton method in general does not converge for all possible choices of $x^{(0)}$, but only for those values of $x^{(0)}$ which are sufficiently close to α . Since we don't know the value of α a possible initial value $x^{(0)}$ can be obtained by resorting to a few iterations of the bisection method or through an investigation of the graph of f .

If $f \in C^2(\mathbb{R})$, $f'(\alpha) \neq 0$, and $x^{(0)}$ is taken sufficiently near α the Newton method converges quadratically. In the case of zeros with multiplicity m larger than one Newton method converges linearly. To avoid this degradation it is possible to use the modified Newton method:

$$x^{(k+1)} = x^{(k)} - m \frac{f(x^{(k)})}{f'(x^{(k)})} \quad k \geq 0$$

provided $f'(x^{(k)}) \neq 0$.

Another modification to this method is the quasi-Newton method that uses a derivative by finite difference:

$$f'(x^{(k)}) \simeq \frac{f(x^{(k)} + h) - f(x^{(k)})}{h}$$

The inputs for the algorithm are: a function $f \in C^1(\mathbb{R})$ and an initial guess $x^{(0)} \in \mathbb{R}$.

Algorithm 2 Algorithm for the basic Newton method

```

1: for  $k = 0, 1, \dots, n$  do
2:    $x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$ 
3:   if  $k > k_{max} \vee |x^{(k)} - x^{(k-1)}| \leq \epsilon_s \vee |f(x^{(k+1)})| \leq \epsilon_r$  then
4:     return  $x^{(k+1)}$ 
5:   end if
6: end for
```

The pros are:

- Fast convergence.
- Works also for zeros with even multiplicity.

The cons are:

- Require computation of the derivative.
- Choice of the right $x^{(0)}$.

2.6 Secant method

For the computation of the zeros of a function f whose derivative is not available in analytical form, the Newton method cannot be applied. However, we should be able to compute the function f at any arbitrary point, and we could replace the exact value $f'(x^{(k)})$ with an incremental ratio based on previously computed values of f . The secant method exploits this strategy and converges super-linearly ($q = 1.6$).

The inputs for the algorithm are: two initial guesses $x^{(0)} \in \mathbb{R}$ and $x^{(1)} \in \mathbb{R}$.

Algorithm 3 Algorithm for the secant method

```

1: for  $k = 0, 1, \dots, n$  do
2:    $x^{(k+1)} = x^{(k)} - f(x^{(k)}) \frac{x^{(k)} - x^{(k-1)}}{f(x^{(k)}) - f(x^{(k-1)})}$ 
3:   if  $k > k_{max} \vee |x^{(k)} - x^{(k-1)}| \leq \epsilon_s \vee |f(x^{(k+1)})| \leq \epsilon_r$  then
4:     return  $x^{(k+1)}$ 
5:   end if
6: end for

```

2.7 Systems of nonlinear equations

2.8 Fixed point method

Given a function $\phi : [a, b] \rightarrow \mathbb{R}$, find $\alpha \in [a, b]$ such that $\alpha = \phi(\alpha)$. If such an α exists it will be called a fixed point of ϕ , and it could be computed by the following algorithm:

$$x^{(k+1)} = \phi(x^{(k)}) \quad k \geq 0$$

where $x^{(0)}$ is an initial guess. This algorithm is called fixed point iteration and ϕ is said to be the iteration function.

Theorem (*Lipschitz continuity*)

1. Let us suppose that $\phi(x)$ is continuous in $[a, b]$ and such that $\phi(x) \in [a, b]$ for every $x \in [a, b]$; then, there exists at least a fixed point $\alpha \in [a, b]$.

2. Moreover, if

$$\exists L < 1 \text{ such that } |\phi(x_1) - \phi(x_2)| \leq L |x_1 - x_2| \quad \forall x_1, x_2 \in [a, b]$$

then there exists a unique fixed point $\alpha \in [a, b]$ of ϕ and the sequence converges to α , for any choice of initial guess $x^{(0)} \in [a, b]$.

Proof of the first proposition :

Proof of the second proposition :

