Numerical methods

Session 1: Principles of numerical mathematics

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Consider the following expression:

$$F(x, d) = 0 \tag{1}$$

in which we call x the unknown, d data and F is the relation between x and d.

1. If F and d are known, finding x will be called the "direct problem".
2. If F and x are known, finding d will be called the "inverse problem".
3. If x and d are known, finding F will be called the "identification problem".

In this course we will study the direct problem.

Definition: We say that a problem is well-posed (or stable) if it admits a unique solution x which depends with continuity from the data.

Definition: We say that a problem is ill-posed if it is not well-posed.

Definition: We say that x depends with continuity from the data if a little change δd in the data produces a small change in the solution δx. Mathematically:

If $F(d + \delta d, x + \delta x) = 0$ then:

$$\forall \eta > 0, \exists K(\eta, d) : \|\delta d\| < \eta \Rightarrow \|\delta x\| \leq K(\eta, d)\|\delta d\| \qquad (2)$$

where K is a constant that depends on η and d.

Example: Find the number of roots of the polynomial $p(x) = x^4 - (2a-1)x^2 + a(a-1)$ (a is the data of the problem). Is easy to check that we have four real roots if $a \geq 1$, two is $a \in [0,1)$ and no real roots if $a < 0$. This is an ill posed problem because the solution does not depend continuously from the data.

Well-posedness and condition number of a problem

Most problems are not so clearly ill posed. To quantify the well/ill posedness of a problem we define:

Definition: Relative condition number

$$K(d) = \sup_{\delta d \in D} \frac{\|\delta x\| / \|x\|}{\|\delta d\| / \|d\|} \tag{3}$$

Definition: Absolute condition number

$$K_{abs}(d) = \sup_{\delta d \in D} \frac{\|\delta x\|}{\|\delta d\|} \tag{4}$$

D is a neighborhood of the origin that denotes the admissible perturbations of the data.

Well-posedness and condition number of a problem

Note: You can use any norm you want.
Definition: We say a problem is "ill-conditioned" if K is "big" where the definition of big depends on the problem.
It is important to understand that the conditioning of a problem does not depend on the algorithm used to solve it. You can develop stable and unstable algorithms for well-posed problems. The concept of stability for algorithms will be defined later on. Having a "big" or even infinite condition number does not imply that the problem is ill-posed. Some ill-posed problems can be reformulated as an equivalent problem (that is, one that has the same solution) which are well-posed.

Well-posedness and condition number of a problem

If a problem admits a unique solution, then there exist a mapping G, called the **resolvent**, between the data and the solutions sets such that:

$$x = G(d), \text{ that is, } F(G(d), d) = 0 \tag{5}$$

According to this, and assuming G is differentiable in d ($G'(d)$ exist), the Taylor expansion of G is

$$G(d + \delta d) - G(d) = G'(d)\delta d + o(\|\delta d\|) \text{ for } \delta d \to 0$$

This let us redefine the condition numbers in terms of the resolvent G:

$$K(D) \approx \|G'(d)\| \frac{\|d\|}{\|G(d)\|} \qquad \text{and} \qquad K_{abs} \approx \|G'(d)\|$$

Example of ill-conditioning: Algebraic second degree equation:

We want to calculate the solutions of $x^2 - 2px + 1$ with $p \geq 1$. Obviously $x_{\pm} = p \pm \sqrt{p^2 - 1}$.
We can formulate this problem as $F(x, p) = x^2 - 2px + 1$ where p is the data and $x_{\pm} = (x_+, x_-)$ the solution. The resolvent $G(p) = (p + \sqrt{p^2 - 1}, p - \sqrt{p^2 - 1})$ and its derivative $G'(p) = (1 + 1/\sqrt{p^2 - 1}, 1 - 1/\sqrt{p^2 - 1})$.

Then:

$$K(d) \approx \|G'(d)\| \frac{\|d\|}{\|G(d)\|} = \frac{(1p^2/(p^2-1)^{1/2})}{(2(p^2-1))^{1/2}} \|p\| = \frac{p}{p^2-1}|p|$$

$$K_{abs}(d) \approx \|G'(d)\| = \sqrt{2}\frac{p}{\sqrt{p^2-1}}$$

If $p >> 1$ then the problem is well-conditioned (two distinct roots). If $p = 1$ (one double root), then G is not differentiable but in the limit $p \to 1^+$ the problem is ill conditioned as $\lim_{p \to 1^+} \|G'(p)\| = \infty$.

However, the problem is not ill-posed. We can reformulate it as $F(x,t) = x^2 - ((1+t^2)/t)x + 1$ with $t = p + \sqrt{p^2-1}$. In this case $x_+ = t$ and $x_- = 1/t$ are the same for $t = 1$, and $K(t) \approx 1 \ \forall t \in \mathbb{R}$

Stability of numerical methods

Let's assume the the problem $F(x, d) = 0$ is well-posed. Then, a numerical method to approximate its solution will consist, in general, of a sequence of approximate problems

$$F_n(x_n, d_n) = 0 \quad n \geq 1$$

We would expect that $x_n \underset{n\to\infty}{\to} x$. For that it is necessary that $d_n \to d$ and that F_n approximates F when $n \to \infty$.

Definition: We say that $F_n(x_n, d_n) = 0$ is consistent if

$$F_n(x, d) = F_n(x, d) - F(x, d) \underset{n\to\infty}{\rightarrow} 0$$

where x is the solution of $F(x, d) = 0$ for the datum d.
Definition: We say that a method is strongly consistent if $F_n(x, d) = 0 \quad \forall n$.
In some cases when iterative methods are used, we can write them as

$$F(x_n, x_{n-1}, \cdots, x_{n-q}, d_n) = 0$$

where $x_n, x_{n-1}, \cdots, x_{n-1}$ are given. In this case the property of strong consistency becomes $F_n(x, x, \cdots, x, d) = 0 \;\; \forall n \geq q$.

Examples:

1. Newton's method: $x_n = x_{n-1} - \frac{f(x_{n-1})}{f'(x_{n-1})}$ is strongly consistent.
2. Composite midpoint rule: If $x = \int_a^b f(t)dt$,
   $x_n = H \sum_{k=1}^{n} f(\frac{t_k + t_{k+1}}{2}) \quad n \geq 1$ with $H = (b-a)/n$ and $t_k = a + (k-1)H$. This method to calculate the integral is consistent, but only strongly consistent if f is a piecewise linear polynomial.
   In general, numerical methods obtained from the mathematical problem by truncation of limit operations (like integrals, derivatives, series,...) are not strongly consistent.

Definition: We say that a numerical method $F_n(x_n, d_n) = 0$ is well-posed (or stable) if for any fixed n there exists a unique solution x_n corresponding to the datum d_n, that the computation of x_n as a function of d_n is unique, and that x_n depends continuously on the data, i.e:

$$\forall \eta > 0, \exists K_n(\eta, d_d) : \|\delta d_n\| < \eta \Rightarrow \|\delta x - n\| \leq K_n(\eta, d_n)\|\delta d_n\| \quad (6)$$

Stability of numerical methods

We can also define:

$$K_n(d_n) = \sup_{\delta d_n \in D_n} \frac{\|\delta x_n\|/\|x_n\|}{\|\delta d_n\|/\|d_n\|} \qquad K_{abs,n}(d_n) = \sup_{\delta d_n \in D_n} \frac{\|\delta x_n\|}{\|\delta d_n\|} \tag{7}$$

and from these:

$$K^{num}(d_n) = \lim_{n\to\infty} \sup_{n\geq k} K_n(d_n) \tag{8}$$

$$K^{num}_{abs}(d_n) = \lim_{n\to\infty} \sup_{n\geq k} K_{abs,n}(d_n) \tag{9}$$

K_{num} is the relative asymptotic condition number and K^{num}_{abs} is the absolute asymptotic condition number of the numerical method corresponding to the datum d_n.
The numerical method is said to be well-conditioned if the condition number K^{num} is "small" for any admissible datum d_n and ill-conditioned otherwise.

Stability of numerical methods

We can also define the resolvent G_n for the numerical method:

$$x_n = G(d_n), \text{ that is } F(G_n(d_n), d_n) = 0$$

Assuming it is differentiable:

$$K_n(d_n) \approx \|G_n'(d_n)\| \frac{\|d_n\|}{\|G_n(d_n)\|} \qquad \text{and} \qquad K_{abs} \approx \|G_n'(d_n)\|$$

Examples:

- Sum and subtraction. The sum defined as

$$f: \underset{(a,b)}{\mathbb{R}^2} \to \underset{a+b}{\mathbb{R}}$$

has derivative $f'(a,b) = (1,1)^T$, and thus, its condition number $K((a,b)) \approx \frac{|a|+|b|}{|a+b|} \approx 1$ The subtraction defined as

$$f: \underset{(a,b)}{\mathbb{R}^2} \to \underset{a-b}{\mathbb{R}}$$

has derivative $f'(a,b) = (1,-1)^T$, and thus, its condition number $K((a,b)) \approx \frac{|a|+|b|}{|a-b|}$ which can be very big if $a \approx b$.

Stability of numerical methods

- Finding the roots of $x^2 - 2px + 1 = 0$ is well-conditioned, but we can develop an unstable algorithm: $x_- = p - \sqrt{p^2 - 1}$ because this formula is subject to errors due to numerical cancellation of digits in the subtraction. The Newton's method could be a stable algorithm to solve this problem:

$$x_n = x_{n-1} - \frac{x_{n-1}^2 - 2px_{n-1} + 1}{2x_{n-1} - 2p}$$

The method's condition number is $K_n(p) = \frac{|p|}{|x_n - p|}$. To compute $K_n^{num}(p)$ we notice that if the algorithm converges, then $x_n \to x_+$ or x_-, therefore, $|x_n - p| \to \sqrt{p^2 - 1}$ and $k_n(p) \to K_n^{num}(p) \approx \frac{|p|}{\sqrt{p^2-1}}$ which is similar to the condition number of the exact problem. Then, if $p \approx 1$ the problem is ill-conditioned.

Definition: We say that the numerical method $F_n(x_n, d_n) = 0$ is convergent if and only if

$$\forall \epsilon > 0 \; \exists n_0(\epsilon), \exists \delta(n_0, \epsilon) : \forall n > n_0, \forall \|\delta d_n\| < \delta(n_0, \epsilon) \Rightarrow$$

$$\|x(d) - x_n(d + \delta d_n)\| < \epsilon$$

where d is an admissible datum, $x(d)$ the corresponding solution, and $x(d + \delta d_n)$ is the solution of the numerical problem $(F_n(x_n, d_n))$ with datum $d + \delta d_n$.

Definition: Absolute and relative errors:

$$E(x_n) = |x - x_n| \qquad E_{rel}(x_n) = \frac{|x - x_n|}{|x|} \quad (x \neq 0)$$

Definition: Error by component:

$$E^c_{rel}(x_n) = \max_{i,j} \frac{|(x - x_n)_{i,j}|}{|x_{i,j}|} \quad (x_{i,j} \neq 0)$$

Relations between stability and convergence

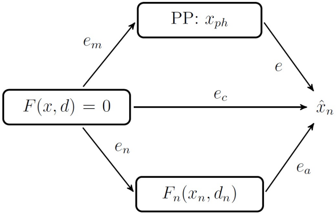
The concepts of stability and convergence are strongly connected. If a (numerical) problem is well-posed, stability is a necessary condition for convergence. Moreover, if the numerical problem is consistent, stability is a sufficient condition for convergence. This is known as "equivalence" or "Lax-Richtmyer" theorem: *For a consistent numerical method, stability is equivalent to convergence*.

Sources of errors in computational models

Whenever the numerical problem (NP) is an approximation of a mathematical problem (MP) and this latter is in turn a model of a physical problem (PP), we say that NP ($F_n(x_n, d_n) = 0$) is a computational model for PP.

The global error $e = |x_{ph} - x_n|$ can be interpreted as the sum of the MP error $e_m = x - x_{ph}$ and the computational problem error $e_c = \hat{x} - x$ ($e = e_m + e_c$).

e_a: Error induced by the numerical algorithm and the rounding errors.



Stability of numerical methods

In general, we can enumerate the following sources of error:

1. Errors due to the model, that can be **reduced** by using a proper model.
2. Errors due to data, that can be **reduced** improving the measurement's accuracy.
3. Truncation errors, arising from the approximation (truncation) of limit operations (integrals, derivatives,...).
4. Rounding errors.

Type 3 and 4 errors give rise to the computational error. A numerical method will be convergent if this error can be made arbitrarily small increasing the computational effort. Although convergence is the primary goal of a numerical method, there are also the accuracy, the reliability and the efficiency.

Accuracy means that the errors are small with respect to a fixed tolerance. It is usually quantified by the infinitesimal order of the error e_n with respect to the discretization characteristic parameter (for example the largest grid spacing).

Note: Machine precision does not limit, theoretically, the accuracy.

Reliability means that it is very likely that the global error is below a certain tolerance.

Efficiency mean that the computational (effort) complexity needed to control the error (number of operation and memory) is as small as possible.

Definition: Algorithm is a directive that indicates, through elementary operations, all the passages needed to solve a problem. It should finish after a finite number of steps, and as a consequence the executor (man or machine) must find within the algorithm itself all the instructions to completely solve the problem.
Complexity of an algorithm is a measure of its executing time.
Complexity of a problem is the complexity of the algorithm with smallest complexity capable of solving the problem.