Validation for scientific computations
Error analysis

Cours de recherche master informatique

Nathalie Revol

Nathalie.Revol@ens-lyon.fr

20 octobre 2006

References for today's lecture

Condition number:

- Ph. Langlois: HDR (LIP, 2001) and chapter in A. Barraud et al.: Outils d'analyse numérique pour l'automatique, Hermes, 2002
- N.H. Higham: Accuracy and stability of numerical algorithms, SIAM, 1996 (1st edition)
- P. Lascaux and R. Théodor: Analyse numérique matricielle appliquée à l'art de l'ingénieur, Masson, 1993 (2nd edition)

Forward and backward analyses:

- Ph. Langlois: HDR (LIP, 2001) and chapter in A. Barraud et al.: Outils d'analyse numérique pour l'automatique, Hermes, 2002
- N.H. Higham: Accuracy and stability of numerical algorithms, SIAM, 1996 (1st edition)
- A. Neumaier: Introduction to numerical analysis, Cambridge University Press, 2001

Definition of well-posed problem and ill-posed problem

Problem $\mathcal{P}$:
compute

$$y = f(x)$$

where x: input, y: output or result.
It can also be given implicitely:

$$F(x, y) = 0 \text{ or } x = F(y).$$

Definition of well-posed problem and ill-posed problem

Well-posed problem $\mathcal{P}$:
$y = f(x)$ exists, is unique and depends continuously of x.
If the problem is given as $x = F(y)$, this means that $F^{-1}(x)$ exists, is unique and F^{-1} is continuous.

If the problem is not well-posed, then it is **ill-posed**.

In what follows, we assume that every problem is well-posed.

Relative error, absolute error

If $\in \mathbb{R}$, $\hat{x}$ is an approximation of x and $\Delta x = \hat{x} - x$
absolute error on x: $|\Delta x| = |\hat{x} - x|$
relative error on x, if $x \neq 0$: $|\frac{\Delta x}{x}| = |\frac{\hat{x}-x}{x}|$

If $x \in \mathbb{R}^n$,
absolute error on x: $\|\Delta x\|_a = \|\hat{x} - x\|$
relative error on x, if $x \neq 0$:

- normwise: $\|\Delta x\|_r = \frac{\|\Delta x\|}{\|x\|} = \frac{\|\hat{x}-x\|}{\|x\|}$
- componentwise: $|\Delta x\|_r = \max_{1 \leq i \leq n} \left| \frac{\Delta x_i}{x_i} \right|$

Definition of condition number

In french: conditionnement ou nombre de condition.

Problem $\mathcal{P}$: compute $y = f(x)$ with

$$\begin{array}{ccccc} f & : & D & \longrightarrow & R \\ & & \|\cdot\|_D & & \|\cdot\|_R \end{array}$$

If x and y do not vanish,

$$\kappa(\mathcal{P}, x) = \lim_{\delta \to 0} \sup_{\frac{\|\Delta x\|_D}{\|x\|_D} \le \delta} \frac{\|\Delta y\|_R / \|y\|_R}{\|\Delta x\|_D / \|x\|_D}$$

Definition of condition number

Problem $\mathcal{P}$: compute $y = f(x)$ with

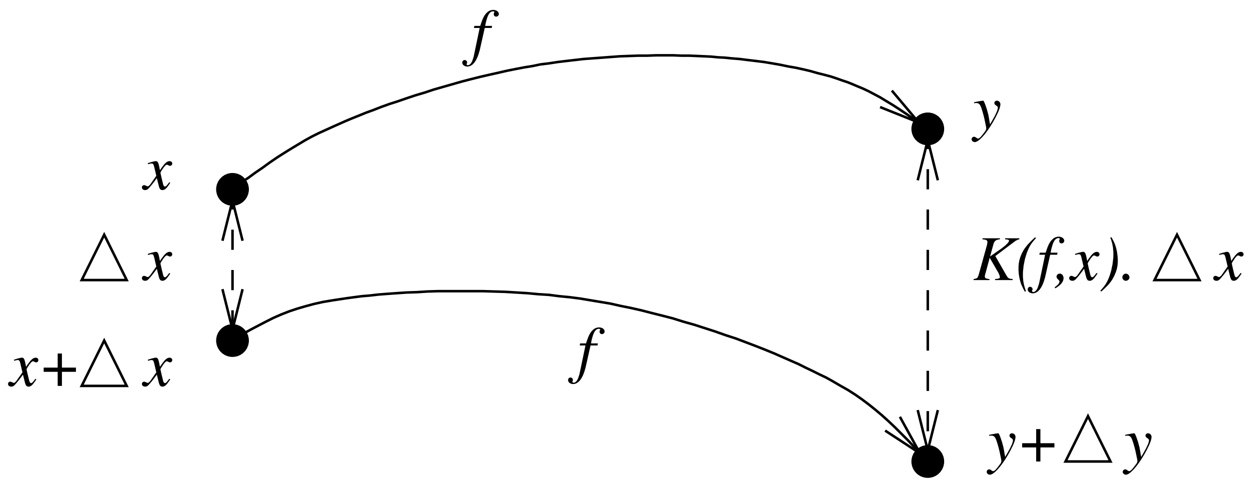
$$\begin{array}{cccc} f & : & D & \longrightarrow & R \\ & & \|.\|_D & & \|.\|_R \end{array}$$

If x or y vanish, one uses absolute errors instead of relative errors and one gets an absolute condition number:

$$\kappa(\mathcal{P}, x) = \lim_{\delta \to 0} \sup_{\|\Delta x\|_D \le \delta} \frac{\|\Delta y\|_R}{\|\Delta x\|_D}$$

Interpretation of condition number

The condition number is the factor of amplification (or reduction) of the error:



Well-conditioned, ill-conditioned problem

A problem is well-conditioned if its condition number is small, i.e., close to 1,
it is ill-conditioned if its condition number is large, i.e., $\gg 1$.

It is a qualitative notion. . .

Condition number: subtraction $y = x_1 - x_2$

Let us consider $\hat{x_1} = x_1(1+\delta_1)$ $\hat{x_2} = x_2(1+\delta_2)$, and $\hat{y} = y + \Delta y = x_1(1+\delta_1) - x_2(1+\delta_2)$, thus

$$\|\Delta y\|_r = \frac{|\Delta y|}{|y|} = \frac{|x_1\delta_1 - x_2\delta_2|}{|x_1 - x_2|} \leq \frac{|x_1| + |x_2|}{|x_1 - x_2|} \max(|\delta_1|, |\delta_2|).$$

If we use the componentwise relative error,

$$\kappa(-, (x_1, x_2)) = \lim_{\delta \to 0} \sup_{x : \|\Delta x\|_r \leq \delta} \frac{|\Delta y| / |y|}{\|\Delta x\|_r} \leq \frac{|x_1| + |x_2|}{|x_1 - x_2|}$$

and there is an equality, when $x_1.x_2 \geq 0$ and when $\delta_1 = -\delta_2$.

Condition number: subtraction $y = x_1 - x_2$

$$\kappa(-, (x_1, x_2)) = \frac{|x_1| + |x_2|}{|x_1 - x_2|}$$

This condition number can be arbitrarily large when x_1 and x_2 are close, i.e., when $|x_1 - x_2| \ll |x_1| + |x_2|$.

This means that, if x_1 and x_2 are computed results with some uncertainty, this uncertainty is magnified by this subtraction:
catastrophic cancellation.

Condition number: subtraction $y = x_1 - x_2$

Cancellation is not always a bad thing:

- no problem when x_1 and x_2 are error-free, cf. divided difference schemes;
- cancellation may be a symptom of intrinsic ill-conditioning and may therefore be unavoidable;
- the result may be harmless, for instance in $(x_1 - x_2) + x_3$ when $x_3 \gg x_1 - x_2$.

Condition number: division $y = x_1/x_2$

Let us consider $\hat{x_1} = x_1(1+\delta_1)$ $\hat{x_2} = x_2(1+\delta_2)$, and $\hat{y} = y + \Delta y = \frac{x_1(1+\delta_1)}{x_2(1+\delta_2)}$, i.e., $\Delta y = \frac{x_1}{x_2}.\frac{\delta_1-\delta_2}{1+\delta_2}$, thus

$$\|\Delta y\|_r = \frac{|\Delta y|}{|y|} = \frac{|\delta_1 - \delta_2|}{|1+\delta_2|} \leq \frac{2\max(|\delta_1|, |\delta_2|)}{1-|\delta_2|}.$$

If we use the componentwise relative error,

$$\kappa(-,(x_1,x_2)) = \lim_{\delta\to 0} \sup_{x:\|\Delta x\|_r \leq \delta} \frac{|\Delta y|/|y|}{\|\Delta x\|_r} \leq 2$$

i.e., the division is always well-conditioned.

Condition number: evaluation of $p(x)$

Let $p(x) = \sum_{i=0}^{n} a_i x^i$ a polynomial.

Let us evaluate $\hat{p}$ in x, where $\hat{p}(x) = \sum_{i=0}^{n} (a_i + \Delta a_i) x^i$:

$$\Delta y = \hat{p}(x) - p(x) = \sum_{i=0}^{n} \Delta a_i x^i$$

and thus

$$\frac{|\Delta y|}{|y|} = \frac{|\sum_{i=0}^{n} \Delta a_i x^i|}{|\sum_{i=0}^{n} a_i x^i|} \leq \frac{\sum_{i=0}^{n} |\Delta a_i|.|x|^i}{|\sum_{i=0}^{n} a_i x^i|} \leq \|\Delta a\|_r \frac{\sum_{i=0}^{n} |a_i|.|x|^i}{|\sum_{i=0}^{n} a_i x^i|}$$

and there is an equality if $\Delta a_i = sign(a_i x^i).\|\Delta a\|_r$.

Condition number: evaluation of $p(x)$

This implies

$$\kappa(p(x), p) = \frac{\sum_{i=0}^{n} |a_i|.|x|^i}{|p(x)|}.$$

In other words, the evaluation of a polynomial p at x can be arbitrarily ill-conditioned when x is close to a root of p.

Condition number: solving the linear system $Ax = b$

$$A = \begin{pmatrix} 10 & 7 & 8 & 7 \\ 7 & 5 & 6 & 5 \\ 8 & 6 & 10 & 9 \\ 7 & 5 & 9 & 10 \end{pmatrix} \quad b = \begin{pmatrix} 32 \\ 23 \\ 33 \\ 31 \end{pmatrix}$$

solution of $Ax = b$: $x = (1\ 1\ 1\ 1)^t$.
If the system is perturbed in

$$A + \Delta A = \begin{pmatrix} 10 & 7 & 8.1 & 7.2 \\ 7.08 & 5.04 & 6 & 5 \\ 8 & 5.98 & 9.89 & 9 \\ 6.99 & 4.99 & 9 & 9.98 \end{pmatrix},$$

the solution of $(A + \Delta A)x = b$ is $(-81\ 137\ -34\ 22)^t$.

Condition number: solving the linear system $Ax = b$

If x is the solution of $Ax = b$ and $\hat{x}$ is the solution of $Ax = b + \Delta b$,

$$\begin{array}{rlcll} & A\Delta x & = & \Delta b & \\ \Rightarrow & \Delta x & = & A^{-1}\Delta b & \\ \Rightarrow & \|\Delta x\| & = & \|A^{-1}\Delta b\| & \leq \|A^{-1}\|.\|\Delta b\| \end{array}$$

We also have

$$\begin{array}{rlcl} & Ax & = & b \\ \Rightarrow & \|Ax\| & = & \|b\| \\ \Rightarrow & \|A\|.\|x\| & \geq & \|b\| \\ \Rightarrow & \frac{\|A\|}{\|b\|} & \geq & \frac{1}{\|x\|} \end{array}$$

and thus $\frac{\|\Delta x\|}{\|x\|} \leq \|A\|.\|A^{-1}\|\frac{\|\Delta b\|}{\|b\|}$

Condition number: solving the linear system $Ax = b$

$$\kappa(A) = \|A\|.\|A^{-1}\|$$

It also holds that, if $x + \Delta x$ is the solution of $(A + \Delta A)x = b$,

$$\frac{\|\Delta x\|}{\|x\|} \leq \kappa(A).\frac{\|\Delta A\|}{\|A\|}$$

and if $x + \Delta x$ is the solution of $(A + \Delta A)x = b + \Delta b$,

$$\frac{\|\Delta x\|}{\|x\|} \leq \frac{\kappa(A)}{1 - \kappa(A).\frac{\|\Delta A\|}{\|A\|}} \left[\frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta b\|}{\|b\|} \right].$$

Condition number: link with a first-order analysis

Problem $\mathcal{P}$: compute $y = f(x)$.

$$y + \Delta y = f(x + \Delta x) \simeq f(x) + f'(x).\Delta x + \mathcal{O}(\Delta x^2)$$

and thus

$$\frac{|\Delta y|}{|y|} \simeq \frac{|f'(x)|.|\Delta x|}{|f(x)|} = \frac{|f'(x)|.|x|}{|f(x)|}.\frac{|\Delta x|}{|x|}$$

i.e.,

$$\kappa(\mathcal{P}, x) \simeq \left| \frac{f'(x).x}{f(x)} \right|.$$

Condition number: link with a first-order analysis

When x and y are not scalars, but vectors: the absolute condition number is

$$\kappa_a(\mathcal{P}, x) = \|f'(x)\|$$

it can also be interpreted as the Lipschitz constant for f',
and the relative condition number is

$$\kappa(\mathcal{P}, x) = \frac{\|f'(x)\|.\|x\|}{\|f(x)\|}.$$

Condition number: remarks

1. the choice of the norms $\|.\|_D$ and $\|.\|_R$ modifies the condition number; the choice of the authorized perturbations Δx as well: one may preserve the structure of the problem and restrict Δx (sparsity of a matrix. . .)

2. quite often, the condition number measures the inverse of the distance to the nearest singular problem (or ill-posed problem)

3. the condition number depends only on the problem $\mathcal{P}$ and not on the algorithm that solves it

4. only small perturbations are considered here, for large perturbations consider interval arithmetic.