Validation for scientific computations
Error analysis: examples

Cours de recherche master informatique

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23 octobre 2006

References for today's lecture

- W. Kahan: How mindless are futile assessments of roundoff errors?
- N.H. Higham: Accuracy and stability of numerical algorithms, SIAM, 1996 (1st edition)

JM Muller's recurrence

Definition of the recurrence:

$$x_{n+1} = 108 - \frac{815 - \frac{1500}{x_n - 1}}{x_n}$$

with $x_0 = 4$ and $x_1 = 4.25$.
Compute x_{80}.

Can You "Count" on Your Computer? up to 6. . . (N. Higham)

$$2 - 1$$

$$\left(\frac{1}{\cos(100\pi + \pi/4)}\right)^2$$

$$3.0 * (tan(atan(10000000.0))/10000000.0)$$

$$\left(\cdots(\sqrt{\cdots\sqrt{4}})^2\cdots\right)^2$$ (20 fois)

$$5 \times \frac{(1+e^{-100})-1}{(1+e^{-100})-1}$$

$$\frac{\ln(e^{6000})}{1000}$$

One, two, three (N. Higham)

$2 - 1$	1.0000000000000000
$\left(\frac{1}{\cos(100\pi+\pi/4)}\right)^2$	2.0000000000001110
$3.0 * (tan(atan(10000000.0))/10000000.0)$	3.0000000030727567

Is this a FLOP?

Four, five, six (N. Higham)

$\left(\cdots(\sqrt{\cdots\sqrt{4}})^2\cdots\right)^2$ (20 fois)	4.0000000006294343
$5 \times \frac{(1+e^{-100})-1}{(1+e^{-100})-1}$	NaN
$\frac{\ln(e^{6000})}{1000}$	$+\infty$

Solving a quadratic equation

Determine the roots of $ax^2 + bx + c = 0$

roots:

$$r_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

What happens if $b^2 \gg |4ac|$?

Solving a quadratic equation

Determine the roots of $ax^2 + bx + c = 0$

roots:

$$r_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

Using $r_1 r_2 = ac$, compute

$$r_1 = \frac{-b - sign(b)\sqrt{b^2 - 4ac}}{2a}$$

and

$$r_2 = \frac{2c}{-b - sign(b)\sqrt{b^2 - 4ac}}$$

Exercise: the goal is to approximate the number π.
It is known that the perimeter of the circle of radius $1/2$ is π, and this perimeter is approximated by the perimeter of the regular polygon with n sides in which this circle is inscribed. Let us denote by U_n the perimeter of this regular polygon. It can be shown that $U_n = \tan \frac{\pi}{n}$.

This implis that the following formulae hold:

$$\begin{cases} U_4 & = & 4 \\ U_{2n} & = & \frac{2U_n}{1+\sqrt{1+\left(\frac{U_n}{n}\right)^2}} & = & \frac{2n\left(\sqrt{n^2+U_n^2}-n\right)}{U_n} \end{cases}$$

If you have to write the algorithm that computes the sequence $V_n = U_{2^n}$ for $n \geq 2$, which formula do you choose? Why?

Solving a quadratic equation

Determine the roots of $ax^2 + bx + c = 0$

roots:

$$r_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}.$$

What happens if $b^2 \simeq 4ac$?

Computing the sample variance

Given n numbers $x_1, \cdots, x_n$.

Mean:

$$\bar{x} = \frac{1}{n} \sum_{n=1}^{n} x_i.$$

Variance:

$$s_n^2 = \frac{1}{n-1} \sum_{n=1}^{n} (x_i - \bar{x})^2.$$

Computing the sample variance

Given n numbers $x_1, \cdots, x_n$.

To avoid compute with two passes, one for the mean and one for the variance, one may compute the variance as:

$$s_n^2 = \frac{1}{n-1} \left(\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2 \right).$$

Computing the sample variance

If the data are $(10000, 10001, 10002)^t$, in single precision, one gets $s_n^2 = 1.0$ with

$$s_n^2 = \frac{1}{n-1} \sum_{n=1}^{n} (x_i - \bar{x})^2$$

and one gets $s_n^2 = 0.0$ with

$$s_n^2 = \frac{1}{n-1} \left(\sum_{i=1}^{n} x_i^2 - \frac{1}{n} \left(\sum_{i=1}^{n} x_i \right)^2 \right).$$

Are either of these reasonable?

Computing the sample variance

Another one-pass formula that accumulates

$$M_k = \frac{1}{k}\sum_{i=1}^{k} x_i \text{ and } Q_k = \sum_{i=1}^{k}(x_i - M_k)^2 = \sum_{i=1}^{k} x_i^2 - \frac{1}{k}\left(\sum_{i=1}^{k} x_i\right)^2.$$

This is done by the following updating formulare:

$$\begin{aligned} M_1 &= x_1 & \qquad M_k &= M_{k-1} + \tfrac{x_k - M_{k-1}}{k} \\ Q_1 &= 0 & \qquad Q_k &= Q_{k-1} + \tfrac{(k-1)(x_k - M_{k-1})^2}{k} \end{aligned}$$

after which $s_n^2 = Q_n/(n-1)$.

This formula has a better numerical quality than the other one-pass algorithm, but less good than that of the two-pass algorithm.

Computing the sample variance

Condition number with componentwise norm:

$$\kappa_C = \lim_{\varepsilon \to 0} \sup\{\frac{|V(x) - V(x + \Delta x)|}{\varepsilon V(x)} \; : \; |\Delta x_i| \leq \varepsilon |x_i|, 1 \leq i \leq n\}.$$

One can show that

$$\kappa_C = 2 \frac{\sum_{i=1}^{n} |x_i - \bar{x}| \times |x_i|}{(n-1)V(x)}.$$

Condition number with global norm:

$$\kappa_N = \lim_{\varepsilon \to 0} \sup \{ \frac{|V(x) - V(x + \Delta x)|}{\varepsilon V(x)} \; : \; \|\Delta x\|_2 \leq \varepsilon \|_2 \}.$$

One can show that

$$\kappa_N = 2 \frac{\|x\|_2}{\sqrt{(n-1)V(x)}} \geq \kappa_C.$$

Influence of the choice of the norm:

$$\kappa_N \geq \kappa_C.$$

Arithmétique flottante

Résolution d'un système linéaire par élimination de Gauss

en arithmétique exacte	en arithmétique flottante avec 3 chiffres décimaux
$\begin{pmatrix} 10^{-4} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$	$\begin{pmatrix} 10^{-4} & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$
$\begin{pmatrix} 10^{-4} & 1 \\ 0 & 1-10^4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2-10^4 \end{pmatrix}$	$\begin{pmatrix} 10^{-4} & 1 \\ 1 & -10^4 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ -10^4 \end{pmatrix}$
$\begin{cases} x_2 = \frac{2-10^4}{1-10^4} = \frac{9998}{9999} \simeq 1 \\ x_1 = \frac{1-x_2}{10^{-4}} = \frac{10000}{9999} \simeq 1 \end{cases}$	$\begin{cases} x_2 = \frac{-10^4}{-10^4} = 1 \\ x_1 = \frac{1-x_2}{10^{-4}} = 0 \end{cases}$

Condition number of this matrix?

$$A = \begin{pmatrix} 10^{-4} & 1 \\ 1 & 1 \end{pmatrix}$$

and its inverse is

$$A^{-1} = \frac{1}{1 - 10^{-4}} \begin{pmatrix} -1 & 1 \\ 1 & -10^{-4} \end{pmatrix}$$

With the norm induced by the infinite norm:

$$\kappa(A) = \|A\|_\infty \|A^{-1}\|_\infty = \frac{1}{1 - 10^{-4}}$$

is very close to 1 and thus excellent.