Contrôle dynamique de méthodes d'approximation

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Numerical accuracy of approximation methods

When an approximation $L(h)$ such that $\lim_{h \to 0} L(h) = L$ is computed, it is affected by:

- a truncation error $e_m(h)$
- a round-off error $e_c(h)$.

$$\text{If } h \text{ decreases, } L(h)\text{: } \begin{array}{|c|c|c|} \multicolumn{3}{r}{e_m(h) \longrightarrow} \\ \hline \text{s} & \text{exponent} & \text{mantissa} \\ \hline \multicolumn{3}{r}{\longleftarrow e_c(h)} \end{array}$$

As long as $e_c(h) < e_m(h)$, decreasing h brings reliable information to the mantissa.

The optimal step is reached when $e_c(h) \approx e_m(h)$.

1. How to determine dynamically the optimal step ?
2. Which digits in the approximation obtained are in common with L ?

Stochastic approach of round-off errors

- the CESTAC method
- the concept of computational zero

$\Rightarrow$ Continuous stochastic arithmetic: $X = (m, \sigma^2)$

$\Rightarrow$ Discrete stochastic arithmetic: $X = (X_1, X_2, ..., X_N)$

Significant digits common to two real numbers

Definition

Let a and b be two real numbers, the number of significant digits that are common to a and b can be defined in $\mathbb{R}$ by

1. for $a \neq b$, $C_{a,b} = \log_{10} \left| \frac{a+b}{2(a-b)} \right|$,
2. $\forall a \in \mathbb{R},\ C_{a,a} = +\infty$.

Example:

if $a = 2.4599976$ and $b = 2.4600012$, then $C_{a,b} \approx 5.8$.

On sequences with a linear convergence

Theorem

Let (I_n) *be a sequence converging linearly to* I*, i.e. which satisfies* $I_n - I = K\alpha^n + o(\alpha^n)$ *where* $K \in \mathbb{R}$ *and* $0 < |\alpha| < 1$*, then*

$$C_{I_n, I_{n+1}} = C_{I_n, I} + \log_{10}\left(\frac{1}{1-\alpha}\right) + o(1).$$

If the convergence zone is reached,
the significant decimal digits common to I_n and I_{n+1}, are those of I, up to $\log_{10}\left(\frac{1}{1-\alpha}\right)$.

If $-1 < \alpha \leq \frac{1}{2}$, then $-1 < \log_2\left(\frac{1}{1-\alpha}\right) \leq 1$.
In this case, the significant bits common to I_n and I_{n+1} are those of I, up to one.

Applications in DSA

Let us assume that the convergence zone is reached.

If $I_n - I_{n+1} = @.0$,
the difference between I_n and I_{n+1} is due to round-off errors.

Further iterations are useless.

Consequently

- the optimal iterate I_{n+1} can be dynamically determined
- if $\alpha \leq \frac{1}{2}$, the exact significant bits of I_{n+1} are those of I, up to one.

F. Jézéquel, *Dynamical control of converging sequences computation*, Applied Numerical Mathematics, 50(2): 147-164, 2004.

Dynamical control of approximation methods

Theorem

Let $L(h)$ be an approximation of order p of L, i.e.

$$L(h) - L = Kh^p + \mathcal{O}\left(h^q\right) \text{ with } 1 \leq p < q,\ K \in \mathbb{R}.$$

If L_n is the approximation computed with the step $\frac{h_0}{2^n}$, then

$$C_{L_n,L_{n+1}} = C_{L_n,L} + \log_{10}\left(\frac{2^p}{2^p - 1}\right) + \mathcal{O}\left(2^{n(p-q)}\right).$$

If the convergence zone is reached and $L_n - L_{n+1} = @.0$, the exact significant bits of L_{n+1} are those of L, up to one.

Control of stochastic operations

Theorem

Let X_i be the approximation in stochastic arithmetic of a mathematical value x_i such that its exact significant bits are those of x_i up to p_i ($i = 1, 2$).

Let $\bigcirc$ be an arithmetical operator: $\bigcirc \in \{+, -, \times, /\}$ and $s\bigcirc$ the corresponding stochastic operator: $s\bigcirc \in \{s+\ , s-\ , s\times\ , s/\}$.

Then the exact significant bits of $X_1\ s\bigcirc\ X_2$ are those of the mathematical value $x_1 \bigcirc x_2$, up to $max(p_1, p_2)$.

- proved for stochastic operations
- used in practice for results obtained in DSA

F. Jézéquel, *Dynamical control of converging sequences computation*, Applied Numerical Mathematics, 50(2): 147-164, 2004.

Dynamical control of integrals on an infinite domain

Let $g = \int_0^\infty \phi(x)dx$ and $g_m = \sum_{j=0}^{m} f_j$ with $f_j = \int_{jL}^{(j+1)L} \phi(x)dx$.

We assume that (g_m) converges linearly to g.

An approximation of each integral can be computed in DSA, such that its exact significant bits are those of f_j, up to 1.

Let G_m be the approximation of g_m computed in DSA.

$\Rightarrow$ the exact significant bits of G_m are those of g_m, up to 1.

$\Rightarrow$ if the convergence zone is reached,
the significant bits common to g_m and g_{m+1} are those of g, up to p.

$\Rightarrow$ if $G_m - G_{m+1} = @.0$,
the exact significant bits of G_{m+1} are those of g, up to $p+1$.

Dynamical control of multiple integrals computation

PhD M. Charikhi, Jan. 2005

$$I = \int_{\Omega} f(\mathbf{x}) d\mathbf{x} \text{ with } \Omega \subset \mathbb{R}^{\mathrm{N}}$$

can be approximated by:

$$Q[f] = \sum_{j=1}^{\nu} a_j f(\mathbf{x_j}) \text{ with } a_j \in \mathbb{R} \text{ and } \mathbf{x_j} \in \Omega.$$

The approximation Q is called cubature formula if $N \geq 2$.

- polynomial-based methods
- Monte Carlo methods

Cubpack, R. Cools et al. 1992
VANI, C.-Y. Chen 1998
CLAVIS, S. Wedner 2000

Approximation using the principle of "iterated integrals"

Computation of 2-dimensional integrals

$$s = \int_a^b \int_{y_1(x)}^{y_2(x)} f(x,y)dxdy = \int_a^b g(x)dx \text{ with } g(x) = \int_{y_1(x)}^{y_2(x)} f(x,y)dy.$$

$\forall x \in [a,b]$, an approximation $G(x)$ can be computed in DSA such that its exact significant bits are those of $g(x)$, up to δ.

Let $S_n = \phi(\{G(x_i)\})$ be the approximation of s computed in DSA and $s_n = \phi(\{g(x_i)\})$.

- $\Rightarrow$ the exact significant bits of S_n are those of s_n, up to δ
- $\Rightarrow$ if the convergence zone is reached, the significant bits common to s_{n-1} and s_n are common with s, up to δ
- $\Rightarrow$ if $S_{n-1} - S_n = @.0$,
  the exact significant bits of S_n are those of s, up to 2δ.

The exact significant bits of the approximation obtained are those of the mathematical value of the integral, up to $N\delta$.

- With Romberg's method, $\delta = 0$.
- With the trapezoidal rule, $N\delta$ represents:
  - one bit if $N \leq 2$
  - one decimal digit if $N \leq 8$.
- With Simpson's rule, $N\delta$ represents one bit if $N \leq 35$.
- With the Gauss-Legendre method with 6 points, $N\delta$ represents one bit if $N \leq 2838$.

Computation of an integral involved in crystallography

$$g(a) = \int_0^{+\infty} f(x)dx,$$

with $f(x) = [\exp(x) + \exp(-x)]^a - \exp(ax) - \exp(-ax)$ and $0 < a < 2$.

$g(5/3) \approx 4.45$ (W. Harrison 1981)
$g(5/3) \approx 4.6262911$ (SIAM review 1996)

$g(a)$ can be expressed as a series expansion:

$$g(a) = \sum_{n=1}^{+\infty} \frac{\Pi_{i=0}^{n-1}(a-i)}{(n!)(2n-a)} - \frac{1}{a}.$$

F. Jézéquel, J.-M. Chesneaux, *Computation of an infinite integral using Romberg's method*, Numerical Algorithms, 36(3): 265-283, 2004.

Several numerical problems may occur in the computation of $g(a)$:

- for high values of x, the computation of $f(x)$ may generate cancellations,
- the upper bound of the integral is infinite,
- the quadrature method used, e.g. Romberg's method, generates both a truncation error and a round-off error.

In order to avoid cancellations, the same expression of the integrand is not used at both bounds of the interval.

$$g(a) \approx \int_0^l f_1(x)dx + \sum_{j=1}^{k} \int_{jl}^{(j+1)l} f_2(x)dx,$$

where
$$f_1(x) = \exp(ax)\left[(1+\exp(-2x))^a - 1 - \exp(-2ax)\right]$$
$$f_2(x) = \exp(ax)u(x) - \exp(-ax),$$
$$u(x) = \lim_{n\to\infty} u_n(x) \text{ with } u_n(x) = \sum_{i=1}^{n-1} \frac{\exp(-2ix)}{i!} \Pi_{j=0}^{i-1}(a-j).$$

Dynamical choice of several parameters:

- n such that $u_n(x) \approx u(x)$
- k such that $\int_l^{kl} f_2(x)dx \approx \int_l^{\infty} f_2(x)dx$
- the number of iterations with Romberg's method

Proposition

One can compute an approximation $G(a)$ such that its exact significant digits are those of $g(a)$, up to $\delta = \log_{10}\left(\frac{2}{1-\exp^{-l\min(a,2-a)}}\right)$.

a	$\delta \approx$		$g(a)$
0.5	0.34	exact:	-1.69442616958795 8E+000
		DSA:	-1.69442616958795E+000
$5/3$	0.39	exact:	4.62629111983995E+000
		DSA:	4.626291119833E+000
1.9999	3.6	exact:	1.99989998677609 2E+004
		DSA:	1.99989997358E+004

The exact significant digits of $G(a)$ are in common with $g(a)$, up to $\lceil\delta\rceil$.

Study of an integral involved in the neutron star theory

$$\tau(\varepsilon, v) = \frac{1}{\omega(\varepsilon)} \int_0^{\frac{\pi}{2}} d\theta \sin(\theta) \int_0^{\infty} dn\, n^2 \int_0^{\infty} dp\, h(n, p, \theta, \varepsilon, v)$$

$(\varepsilon, v) \in [10^{-4}, 10^4] \times [10^{-4}, 10^3]$

ω is a normalization function

$$\begin{aligned} h(n, p, \theta, \varepsilon, v) = \quad & \psi(z)\Gamma(n - \varepsilon - z) + \psi(-z)\Gamma(n - \varepsilon + z) \\ & -\psi(z)\Gamma(n + \varepsilon - z) - \psi(z)\Gamma(n + \varepsilon + z) \end{aligned}$$

with $z = \sqrt{p^2 + (v \sin(\theta))^2}$, $\psi(x) = \frac{1}{\exp(x)+1}$, $\Gamma(x) = \frac{x}{\exp(x)-1}$.

F. Jézéquel, F. Rico, J.-M. Chesneaux, M. Charikhi, *Reliable computation of a multiple integral involved in the neutron star theory*, submitted to “Mathematics and Computers in Simulation”.

The numerical problems:

- two infinite bounds
  $\int_0^\infty \ldots$ is replaced by $\sum_{j=0}^{k} \int_{jL}^{(j+1)L} \ldots$
  $\Rightarrow$ Dynamical choice of k
- $\Gamma(x) = \frac{x}{\exp(x)-1}$ generates cancellations if $x \approx 0$.
  a series expansion of $\Gamma(x)$ is used: $\Gamma(x) \approx \frac{1}{1+\frac{x}{2}+\ldots+\frac{x^{n-1}}{n!}}$
  $\Rightarrow$ Dynamical choice of n
- With the principle of “iterated integrals”, the Gauss-Legendre method is used and generates both a truncation error and a round-off error
  $\Rightarrow$ Dynamical control of the Gauss-Legendre method

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$\tau(\varepsilon, v)$ has been computed using DSA in single precision for 5752 points (ε, v) defined by:

$$\left\{ \begin{array}{lllll} \varepsilon & = & 10^a & \textit{with} & a = -4.0, -3.9, -3.8, \ldots, 4.0 \\ v & = & 10^b & \textit{with} & b = -4.0, -3.9, -3.8, \ldots, 3.0. \end{array} \right.$$

The run time of the code varies from 45 s to 3347 s depending on the values of ε and v, the average run time being 389 s.

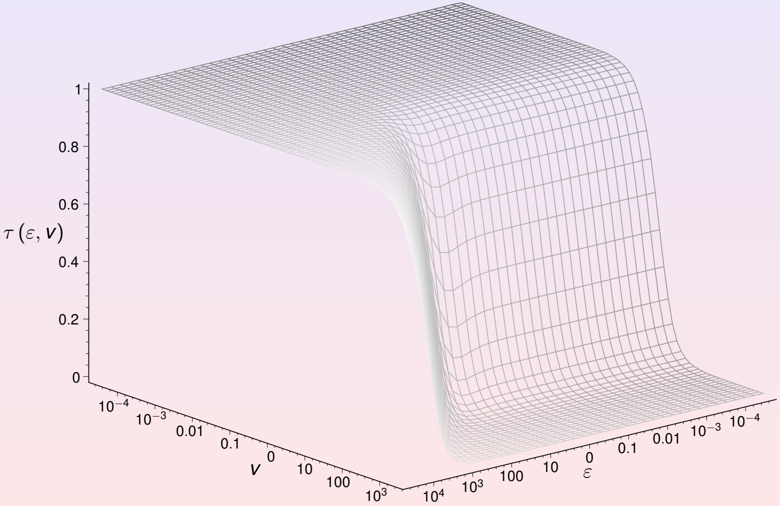
Proposition

One can compute an approximation of $\tau(\varepsilon, v)$ such that its exact significant digits are those of $\tau(\varepsilon, v)$, up to 2.

nb. of exact significant digits	occurrence
3	1
4	217
5	665
6	3347
7	1522

$\Rightarrow$ we can guarantee 1 to 5 significant digits in the results obtained.

Study of an integral involved in the neutron star theory
Numerical results



Conclusion and perspectives - 1/2

Dynamical control of converging sequences computation

Let $u = \lim_{n \to \infty} u_n$. From two iterates in the convergence zone, one can determine the first digits of u.

If $u_n - u_{n+1} = @.0$, one can determine which significant digits of u_{n+1} are in common with u.

Combination of theoretical results if several sequences are involved

For the approximation of an integral, one has to take into account:

- the dimension of the integral
- the number of improper bounds
- the possible approximation of the integrand by its series expansion
- the convergence speed of the sequences involved

Conclusion and perspectives - 2/2

- Adaptive strategies
- Other approximation methods
- Approximation of multiple integrals
  - other cubature methods
  - singular integrals
  - Monte Carlo methods
- Dynamical control of vector sequences computation
  PhD R. Adout
  - acceleration of the restarted GMRES method
  - dynamical control of the dimension of the Krylov subspace
- Automatic methods for round-off error analysis
  - DSA for MATLAB
  - compiler with DSA features
  - linear algebra library
  - grid computing: new methodologies