Floating-point arithmetic and error analysis (AFAE)

Increasing the accuracy, examples with polynomials

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Outline

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1. Floating-point arithmetic
2. Error analysis and increase of accuracy
3. Summation algorithms
4. Dot product algorithms
5. Polynomial evaluation algorithms

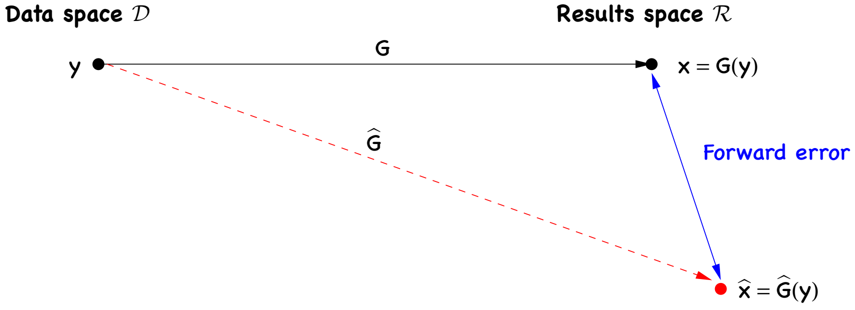
Understanding the difficulties when computing with finite precision

- Controlling the effects of finite precision:
  - How to measure the difficulty of solving the problem?
  - How to characterize the reliability of the algorithm?
  - How to estimate the accuracy of the computed solution?
- Limiting the effects of finite precision
  - How to improve the accuracy of the solution?

How to answer these questions?

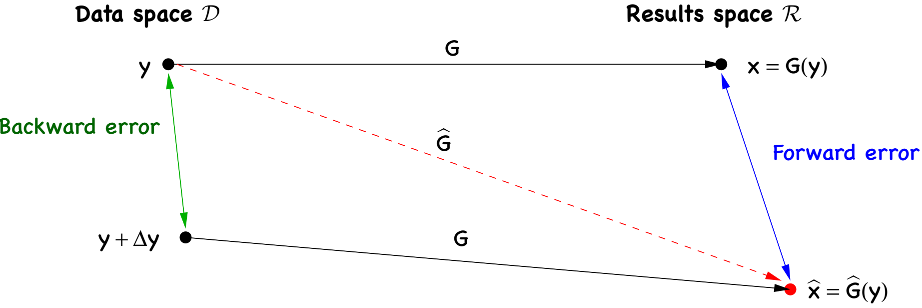
Outline

Error analysis (Wilkinson, Higham)



- Forward error analysis

Error analysis (Wilkinson, Higham)



- Forward error analysis
- Backward error analysis
  Identify $\widehat{x}$ as the solution of a perturbed problem:
  $\widehat{x} = G(y + \Delta y)$.

Advantages of backward error analysis

- **How to measure the difficulty of solving the problem ?** Condition number measures the sensitivity of the solution to perturbation in the data

Condition number : $\mathrm{cond}(P, y) := \lim_{\varepsilon \to 0} \sup_{\|\Delta y\| \leq \varepsilon} \left\{ \frac{\|\Delta x\|_{\mathcal{R}}}{\|\Delta y\|_{\mathcal{D}}} \right\}$

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- **How to appreciate the reliability of the algorithm?**
  Backward error measures the distance between the problem we solved and the initial problem.

  Backward error : $\eta(\widehat{x}) = \min_{\Delta y \in \mathcal{D}} \{\|\Delta y\|_{\mathcal{D}} : \widehat{x} = G(y + \Delta y)\}$

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  At first order, the rule of thumb:

  forward error $\lesssim$ condition number $\times$ backward error.

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Achieving more accuracy with compensated algorithms

Key tools for accurate computation

- fixed length expansions libraries: double-double (Briggs, Bailey, Hida, Li), quad-double (Bailey, Hida, Li)
- arbitrary length expansions libraries: Priest, Shewchuk
- arbitrary multiprecision libraries: MP, MPFUN/ARPREC, MPFR
- compensated algorithms (e.g. Kahan, Priest, Ogita-Rump-Oishi)

Error-free transformations (EFT) (Dekker, Knuth) are properties and algorithms to compute the elementary rounding errors,

$$a, b \in \mathbb{F}, \quad a \circ b = \mathrm{fl}(a \circ b) + e, \text{ and } e \in \mathbb{F}$$

EFT for the summation

$$x = a \oplus b \quad \Rightarrow \quad a + b = x + y \quad \text{with } y \in \mathbb{F},$$

Algorithms of Dekker (1971) and Knuth (1974)

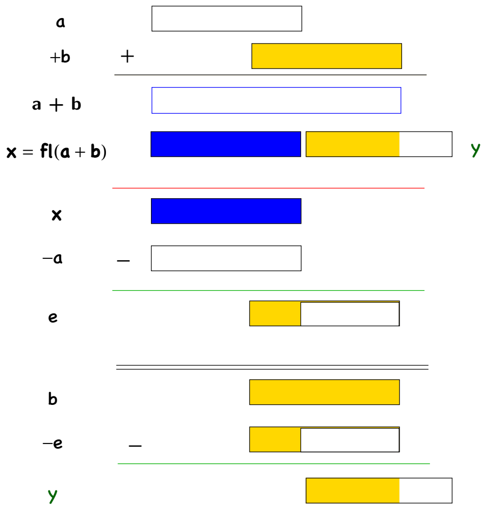
Algorithm (EFT of the sum of 2 floating-point numbers with $|a| \geq |b|$)

function $[x, y]$ = $\texttt{FastTwoSum}(a, b)$
    $x = a \oplus b$
    $y = (a \ominus x) \oplus b$

Algorithm (EFT of the sum of 2 floating-point numbers)

function $[x, y]$ = $\texttt{TwoSum}(a, b)$
    $x = a \oplus b$
    $z = x \ominus a$
    $y = (a \ominus (x \ominus z)) \oplus (b \ominus z)$

EFT for the summation



Error bound for EFT of the sum

Theorem

Let $a, b \in \mathbb{F}$ and let $x, y \in \mathbb{F}$ such that $[x, y] = \mathtt{TwoSum}(a, b)$. Then,

$$a + b = x + y, \quad x = a \oplus b, \quad |y| \leq \mathbf{u}|x|, \quad |y| \leq \mathbf{u}|a + b|.$$

The algorithm `TwoSum` requires 6 flops.

$$x = a \otimes b \quad \Rightarrow \quad a \cdot b = x + y \quad \text{with } y \in \mathbb{F},$$

Algorithm `TwoProduct` by Veltkamp and Dekker (1971)

$$a = x + y \quad \text{and} \quad x \text{ and } y \text{ non overlapping with } |y| \le |x|.$$

Algorithm (Error-free split of a floating-point number into two parts)

function $[x, y]$ = `Split`(a)
  factor = $2^s + 1$ % $u = 2^{-p}$, $s = \lceil p/2 \rceil$
  $c = \texttt{factor} \otimes a$
  $x = c \ominus (c \ominus a)$
  $y = a \ominus x$

EFT for the product (2/3)

Algorithm (EFT of the product of 2 floating-point numbers)

function $[x, y]$ = $\mathtt{TwoProduct}(a, b)$

$x = a \otimes b$

$[a_1, a_2]$ = $\mathtt{Split}(a)$

$[b_1, b_2]$ = $\mathtt{Split}(b)$

y = $a_2 \otimes b_2 \ominus (((x \ominus a_1 \otimes b_1) \ominus a_2 \otimes b_1) \ominus a_1 \otimes b_2)$

Theorem

Let $a, b \in \mathbb{F}$ and let $x, y \in \mathbb{F}$ such that $[x, y] = \mathtt{TwoProduct}(a, b)$. Then,

$$a \cdot b = x + y, \quad x = a \otimes b, \quad |y| \leq \mathbf{u}|x|, \quad |y| \leq \mathbf{u}|a \cdot b|,$$

The algorithm $\mathtt{TwoProduct}$ requires 17 flops.

EFT for the product (3/3)

$$x = a \otimes b \quad \Rightarrow \quad a \times b = x + y \quad \text{with } y \in \mathbb{F},$$

Given $a, b, c \in \mathbb{F}$,

- $\mathrm{FMA}(a, b, c)$ is the nearest floating-point number $a \cdot b + c \in \mathbb{F}$

Algorithm (EFT of the product of 2 floating-point numbers)

function $[x, y]$ = $\mathrm{TwoProduct}(a, b)$

$x = a \otimes b$

$y = \mathrm{FMA}(a, b, -x)$

The FMA is available for example on PowerPC, Itanium, Cell, Xeon Phi, Haswell processors.

Outline

Recursive summmation algorithm

Computation of $s = \sum_{i=1}^{n} p_i$

Algorithm (Classic summation algorithm)

function $\texttt{res}$ = $\mathrm{Sum}(p)$

$\sigma = 0;$

for $i = 1 : n$

$\sigma = \sigma \oplus p_i$

$\texttt{res} = \sigma$

Rounding error analysis(1/2)

Lemma 1

If $|\delta_i| \leq \mathbf{u}$, $\rho_i = \pm 1$ for $i = 1 : n$ and $nu < 1$ then

$$\prod_{i=1}^{n} (1 + \delta_i)^{\rho_i} = 1 + \delta_n,$$

where

$$|\delta_n| \leq \frac{nu}{1 - nu} =: \gamma_n.$$

Rounding error analysis (2/2)

Theorem

With the previous notations, we have

$$|\mathtt{res} - s| \leq \gamma_{n-1} \sum_{i=1}^{n} |p_i|.$$

Kahan's compensated summation algorithm

Algorithm (Kahan's algorithm)

function $\mathtt{res} = \mathtt{SCompSum}(p)$

$\sigma = 0$

$e = 0$

for $i = 1 : n$

$y = p_i \oplus e$

$[\sigma, e] = \mathtt{FastTwoSum}(\sigma, y)$

$\mathtt{res} = \sigma$

Rounding error analysis

Theorem

With the previous notations, we have

$$|\mathrm{res} - s| \le (2u + \mathcal{O}(nu^2)) \sum_{i=1}^{n} |p_i|.$$

Priest's doubly compensated summation algorithm

Algorithm (Priest's algorithm)

function $\mathtt{res} = \mathrm{DCompSum}(p)$
  sort the p_i such that $|p_1| \geq |p_2| \geq \cdots \geq |p_n|$
  $s = 0$
  $c = 0$
  for $i = 1 : n$
    $[y, u] = \mathtt{FastTwoSum}(c, p_i)$
    $[t, v] = \mathtt{FastTwoSum}(s, y)$
    $z = u \oplus v$
    $[s, c] = \mathtt{FastTwoSum}(t, z)$
  $\mathtt{res} = s$

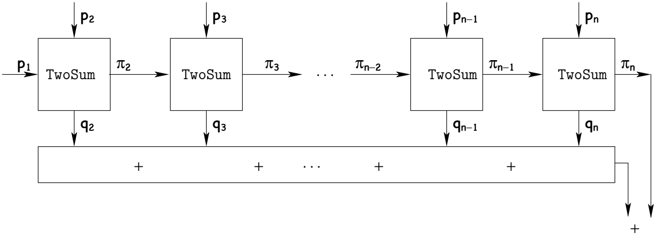
Rounding error analysis

Theorem

With the previous notations, we have

$$|\mathtt{res} - \mathbf{s}| \leq \mathbf{2u}|\mathbf{s}|$$

Compensated algorithm of Ogita, Rump and Oishi



Compensated algorithm of Ogita, Rump and Oishi

Algorithm (Compensated algorithm)

function res = CompSum(p)
  $\pi_1 = p_1$; $\sigma_1 = 0$;
  for $i = 2 : n$
    $[\pi_i, q_i] = \mathrm{TwoSum}(\pi_{i-1}, p_i)$
    $\sigma_i = \sigma_{i-1} \oplus q_i$
  $\mathrm{res} = \pi_n \oplus \sigma_n$

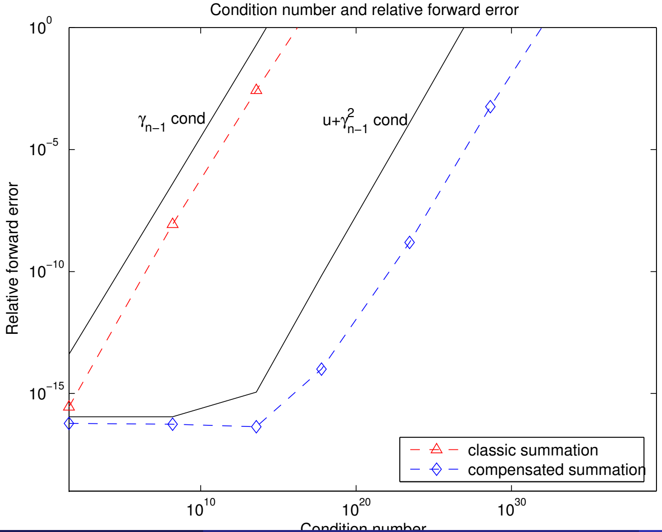
Compensated algorithm of Ogita, Rump and Oishi

Proposition

Let us apply CompSum Algorithm to $p_i \in \mathbb{F}$, $1 \leq i \leq n$. Let $s := \sum p_i$, $S := \sum |p_i|$ and $n\mathbf{u} < 1$. Then, we have

$$|\mathrm{res} - s| \leq \mathbf{u}|s| + \gamma_{n-1}^2 S. \quad (1)$$

Compensated algorithm of Ogita, Rump and Oishi



Outline

Compensated dot product (1/2)

Algorithm (Compensated dot product algorithm)

function $\texttt{res} = \mathrm{CompDot}(x, y)$
  for $i = 1 : n$
    $[r_i, r_{n+i}] = \mathrm{TwoProduct}(x_i, y_i)$
  $\texttt{res} = \mathrm{CompSum}(\mathbf{r})$

Compensated dot product (2/2)

Algorithm (Compensated dot product algorithm)

function $\mathtt{res} = \mathtt{CompDot2}(x, y)$
  $[p, s] = \mathtt{TwoProduct}(x_1, y_1)$
  for $i = 2 : n$
    $[h, r] = \mathtt{TwoProduct}(x_i, y_i)$
    $[p, q] = \mathtt{TwoSum}(p, h)$
    $s = s \oplus (q \oplus r)$
  end
  $\mathtt{res} = p \oplus s$

Proposition

Let floating point numbers $x_i, y_i \in \mathbb{F}$, $1 \le i \le n$, be given and denote by $\mathtt{res} \in \mathbb{F}$ the result computed by Algorithm $\mathtt{CompDot2}$. Then

$$|\mathtt{res} - x^T y| \le u|x^T y| + \gamma_n^2 |x^T||y|.$$

Outline

Horner scheme

Algorithm

function $\mathtt{res} = \mathtt{Horner}(p, x)$ $\qquad$ % $p(x) = \sum_{i=0}^{n} a_i x^i$

$s_n = a_n$

for $i = n-1 : -1 : 0$

$\quad p_i = s_{i+1} \otimes x$

$\quad s_i = p_i \oplus a_i$

end

$\mathtt{res} = s_0$

Condition number for the evaluation of $p(x)$:

$$\mathrm{cond}(p, x) = \frac{\sum_{i=0}^{n} |a_i||x|^i}{|\sum_{i=0}^{n} a_i x^i|} = \frac{\widetilde{p}(|x|)}{|p(x)|}$$

Relative error bound: $$\frac{|p(x) - \mathtt{Horner}(p, x)|}{|p(x)|} \leq \underbrace{\gamma_{2n}}_{\approx 2nu} \mathrm{cond}(p, x)$$

Horner scheme

Algorithm

function $\mathtt{res} = \mathtt{Horner}(p, x)$ % $p(x) = \sum_{i=0}^{n} a_i x^i$

$s_n = a_n$

for $i = n-1 : -1 : 0$

$p_i = s_{i+1} \otimes x$ % rounding error π_i

$s_i = p_i \oplus a_i$ % rounding error σ_i

end

$\mathtt{res} = s_0$

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Relative error bound: $$\frac{|p(x) - \mathtt{Horner}(p, x)|}{|p(x)|} \le \underbrace{\gamma_{2n}}_{\approx 2nu} \mathrm{cond}(p, x)$$

EFT for Horner scheme

Algorithm

function $[\mathtt{Horner}(p,x), p_\pi, p_\sigma] = \mathtt{EFTHorner}(p,x)$

$s_n = a_n$

for $i = n-1 : -1 : 0$

  $[p_i, \pi_i] = \mathtt{TwoProduct}(s_{i+1}, x)$

  $[s_i, \sigma_i] = \mathtt{TwoSum}(p_i, a_i)$

end

$\mathtt{Horner}(p,x) = s_0$

$$p_\pi(x) = \sum_{i=0}^{n-1} \pi_i x^i, \qquad p_\sigma(x) = \sum_{i=0}^{n-1} \sigma_i x^i$$

$$\boxed{p(x) = \mathtt{Horner}(p,x) + (p_\pi + p_\sigma)(x)}$$

Compensated Horner scheme (CHS) and its accuracy

Algorithm (CHS)

function $\texttt{res} = \texttt{CompHorner}(p, x)$
$[h, p_\pi, p_\sigma] = \texttt{EFTHorner}(p, x)$
$c = \texttt{Horner}(p_\pi \oplus p_\sigma, x)$
$\texttt{res} = h \oplus c$

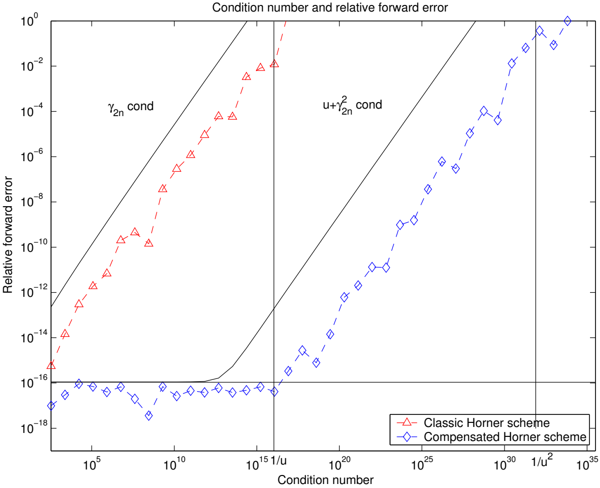
Theorem

Let p be a polynomial of degree n with floating-point coefficients, and x be a floating-point value. Then if no underflow occurs,

$$\frac{|\texttt{CompHorner}(p, x) - p(x)|}{|p(x)|} \leq u + \underbrace{\gamma_{2n}^2}_{\approx 4n^2u^2} \operatorname{cond}(p, x).$$

Numerical experiments: testing the accuracy

Evaluation of $p_n(x) = (x-1)^n$ for $x = \mathrm{fl}(1.333)$ and $n = 3, \ldots, 42$



Numerical experiments: testing the speed efficiency

We compare

- Horner: IEEE 754 double precision Horner scheme
- CompHorner: Compensated Horner scheme
- DDHorner: Horner scheme with internal double-double computation

All computations are performed in C and IEEE 754 double precision

ratio	minimum	mean	maximum	theoretical
CompHorner/Horner	1.5	2.9	3.2	13
DDHorner/Horner	2.3	8.4	9.4	17

Compensated Horner Derivative algorithm

The Horner Derivative (HD) algorithm is the classic method for the evaluation of the k-derivative of a polynomial $p(x)$

Algorithm (HD)

function res=HD(p, x, k)
  $y_i^j = 0$ for $i = 0 : 1 : k$ and $j = n+1 : -1 : 0$
  $y_{-1}^{j+1} = a_j$ for $j = n : -1 : 0$

  for $j = n : -1 : 0$
    for $i = \min(k, n-j) : -1 : \max(0, k-j)$
      $y_i^j = x \otimes y_i^{j+1} \oplus y_{i-1}^{j+1}$
    end
  end
  res $= k! \otimes y_k^0$

Algorithm (CHD)

function res=CompHD(p, x, k)
  $y_i^j = 0$, $\widehat{\varepsilon y}_i^j = 0$, for $i = 0 : 1 : k$, and $j = n+1 : -1 : 0$
  $y_{-1}^{j+1} = a_j$, $\widehat{\varepsilon y}_{-1}^{j+1} = 0$, for $j = n : -1 : 0$
  for $j = n : -1 : 0$
    for $i = \min(k, n-j) : -1 : \max(0, k-j)$
      $[s, \pi_i^j] =$ TwoProd$(x, \widehat{y}_i^{j+1})$
      $[\widehat{y}_i^j, \sigma_i^j] =$ TwoSum$(s, \widehat{y}_{i-1}^{j+1})$
      $\widehat{\varepsilon y}_i^j = x \otimes \widehat{\varepsilon y}_i^{j+1} \oplus \widehat{\varepsilon y}_{i-1}^{j+1} \oplus (\pi_i^j \oplus \sigma_i^j)$
    end
  end
  res $= (\widehat{y}_k^0 \oplus \widehat{\varepsilon y}_k^0) \otimes k!$

Rounding error analysis of CHD algorithm

Theorem

Let $p(x) = \sum_{i=0}^{n} a_i x^i$ be a polynomial of degree n with floating-point coefficients, and x a floating-point value (with $p^{(k)}(x) \neq 0$). The relative forward error bound in CHD algorithm is such that

$$\frac{|\mathrm{CompHD}(p, x, k) - p^{(k)}(x)|}{|p^{(k)}(x)|} \leq 2u + (k+1)\underbrace{\gamma_{2n}\gamma_{3n}}_{\approx 6n^2u^2}\mathrm{cond}(p, x, k).$$

The condition number for the k-th derivative evaluation of a polynomial $p(x) = \sum_{i=0}^{n} a_i x^i$ at entry x is given by

$$\mathrm{cond}(p, x, k) = \frac{k! \sum_{m=k}^{n} \binom{m}{k} |x|^{m-k} |a_m|}{|k! \sum_{m=k}^{n} \binom{m}{k} x^{m-k} a_m|} = \frac{\widetilde{p}^{(k)}(x)}{|p^{(k)}(x)|},$$

Numerical experiments

Average ratios of the floating-point operations

$\frac{\text{CompHD}}{\text{HD}}$	$\frac{\text{DDHD}}{\text{HD}}$	$\frac{\text{CompHD}}{\text{DDHD}}$
8.35	13.60	61%

Measured running time ratios

	$\frac{\text{CompHD}}{\text{HD}}$	$\frac{\text{DDHD}}{\text{HD}}$	$\frac{\text{CompHD}}{\text{DDHD}}$
Linux gcc 4.4.5	3.85	8.14	47%
Windows Vc++9.0	4.58	9.79	47%

Condition number for root finding

Definition

Let $p(z) = \sum_{i=0}^{n} a_i z^i$ be a polynomial of degree n and x be a simple zero of p. The condition number of x is defined by

$$\mathrm{cond}_{\mathrm{root}}(p, x) = \lim_{\varepsilon \to 0} \sup \left\{ \frac{|\Delta x|}{\varepsilon |x|} : |\Delta a_i| \leq \varepsilon |a_i| \right\}.$$

Theorem

Let $p(z) = \sum_{i=0}^{n} a_i z^i$ be a polynomial of degree n and x be a simple zero of p. The condition number of x is given by

$$\mathrm{cond}_{\mathrm{root}}(p, x) = \frac{\widetilde{p}(|x|)}{|x||p'(x)|},$$

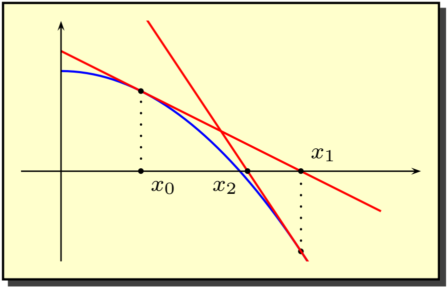
with $\widetilde{p}(x) = \sum_{i=0}^{n} |a_i| z^i$.

Application to Newton's method

Algorithm (The classic Newton's method)

$$x_0 = \xi$$
$$x_{i+1} = x_i - \frac{\mathrm{Horner}(p, x_i)}{\mathrm{HD}(p, x_i, 1)}$$

$$\frac{|x_{i+1} - x|}{|x|} \approx \gamma_{2n}\, \mathrm{cond}_{\mathrm{root}}(p, x) \qquad \text{[Higham, 1996]}$$



Application to Newton's method

Algorithm (The accurate Newton's method)

$$x_0 = \xi$$
$$x_{i+1} = x_i - \frac{\texttt{CompHorner}(p,x_i)}{\texttt{HD}(p,x_i,1)}$$

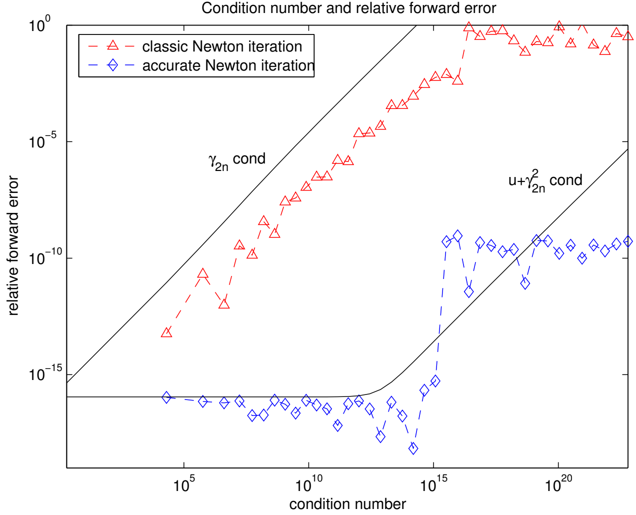
Theorem

Assume that there is an x such that $p(x) = 0$ and $p'(x) \neq 0$ is not too small. Assume also that $\mathbf{u} \cdot \mathtt{cond}_{\mathtt{root}}(p,x) \leq 1/8$. Then, for all x_0 such that $\beta |p'(x)^{-1}| |x_0 - x| \leq 1/8$, Newton's method in floating-point arithmetic generates a sequence of $\{x_i\}$ whose relative error decreases until the first i for which

$$\frac{|x_{i+1} - x|}{|x|} \approx \mathbf{u} + \gamma_{2n}^2 \, \mathrm{cond}_{\mathtt{root}}(p,x).$$

Application to Newton's method

Test with $p_n(x) = (x-1)^n - 10^{-8}$ and $x = 1 + 10^{-8/n}$ for $n = 1 : 40$
$\mathrm{cond}(p_n, x)$ varies from 10^4 to 10^{22}



Application to Newton's method

Algorithm (The new accurate Newton's method)

$$x_0 = \xi$$
$$x_{i+1} = x_i - \frac{\texttt{CompHorner}(p, x_i)}{\texttt{CompHD}(p, x_i, 1)}$$

It is proved that

- that the convergence of iterations strongly depends on the accuracy of the derivative's evaluation when the problem of finding simple root is too ill-conditioned, and
- that the accuracy of the final iteration result depends on the accuracy with which the residual is computed.

Application to Newton's method

It is shown that

In case of classic Newton's algorithm:

$$\left|\frac{x_i - x}{x}\right| < C\gamma_{2n}\mathrm{cond}_{\mathrm{root}}(p, x).$$

In case of accurate Newton's algorithms:

$$\left|\frac{x_i - x}{x}\right| < Ku + D\gamma_{2n}^2\mathrm{cond}_{\mathrm{root}}(p, x).$$

where C, K and D are small factors.

Application to Newton's method

Assume that the simple root is α such that $f(\alpha) = 0$, $f'(\alpha) \neq 0$ with f is continuously differentiable in a neighborhood of the root, and in floating point arithmetic the computation of the derivative satisfies

Assumption 1 : $$\left|\frac{\widehat{f'}(v) - f'(v)}{f'(v)}\right| < \omega < \frac{1}{2},$$

Assume also that for any v, obtained from the iteration from the initial value v_0 sufficiently close to the root α, satisfies

Assumption 2 : $$0 < \frac{f(v)}{f'(v)(v-\alpha)} < \mu_1.$$

In the iterative process, $f'(v) \neq 0$ and $\widehat{f'}(v) \neq 0$, meanwhile ω and μ_1 satisfy

Assumption 3 : $$\mu_1 + 2\omega \leq 2.$$

Application to Newton's method

Newton's method or its improved versions in floating point arithmetic generates a sequence $\{\widehat{v}_i\}$ converging to v_*. Then assume that, when the iteration converges, there is

Assumption 4 : $$0 < \mu_2 < \frac{f(v_*)}{f'(v_*)(v_* - \alpha)}.$$

The parameters ω, μ_1 and μ_2 used in Assumption 1-4 will help to obtain the accuracies guaranteed by the algorithms as follows.
In case of classic Newton's algorithm:

$$\left|\frac{\alpha - v_*}{v_*}\right| < C\gamma_{2n}\mathrm{cond}_{\mathrm{root}}(p, v_*).$$

Application to Newton's method

In case of accurate Newton's algorithms:

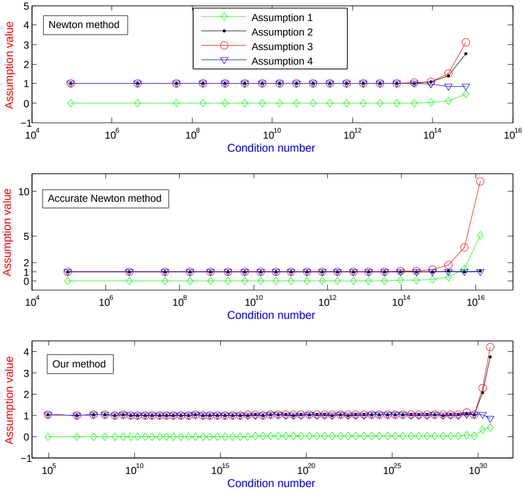
$$\left|\frac{\alpha - v_*}{v_*}\right| < Ku + D\gamma_{2n}^2 \mathrm{cond}_{\mathrm{root}}(p, v_*).$$

where C, K and D are the constants consist of ω and μ_2.

Numerical experiments

- Computing the simple real zero of the expanded form of the polynomial $p_n(x) = (x-1)^n - 2^{-31}$, for $n = 2 : 55$, the condition number of which varies roughly from 10^4 to 10^{32} at the real zero
- If n is even, there are two real roots: $1 \pm 2^{-31/n}$; if n is odd, there is only one real root $1 + 2^{-31/n}$
- We set the initial value $v_0 = 2$, then considering the local convergence property of Newton method, we deem that the iteration sequence will converge to the real root $\alpha = 1 + 2^{-31/n}$
- Stopping criterion $|\widehat{v}_{k+1} - \widehat{v}_k| < tol = 10^{-15}$ and maximum admissible number of steps for the iterative process as $Num = 100$.

Numerical experiments



Assumption values of three algorithms with respect to condition number. Here, Assumption 1 and 2 represent the largest $|\widehat{f'}(v) - f'(v)/f'(v)|$ and the largest $f(v)/f'(v)(v - \alpha)$ for all of the iterates v with respect to some condition number, respectively; Assumption 3 represents the summation of Assumption 2 and double Assumption 1; Assumption 4 represents the smallest $f(v_*)/f'(v_*)(v_* - \alpha)$ with respect to some condition number

Numerical experiments

Simple real zero of the expanded form of the polynomial $p_n(x) = (x-1)^n - 2^{-31}$, for $n = 2 : 55$