Accurate simple zeros of polynomials

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Aim of the talk

- Use Newton's method to accurately compute the simple roots of a polynomial.
- This needs to accurately calculate the residual (*i.e.* to accurately evaluate a polynomial)

Outline of the talk

1. Accurate polynomial evaluation

2. Accurate Newton's method

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What are Error-Free Transformations (EFT) ?

Assume floating point arithmetic adhering IEEE 754 with rounding to nearest with rounding unit $\mathbf{u}$ (no underflow nor overflow)

Error free transformations are properties and algorithms to compute the generated elementary rounding errors,

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

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
- compensated algorithms (Kahan, Priest, Ogita-Rump-Oishi, Graillat-Langlois-Louvet)

EFT for the summation

$$x = \mathrm{fl}(a \pm b) \quad \Rightarrow \quad a \pm b = x + y \quad \text{with } y \in \mathbb{F},$$

Algorithms of Dekker (1971) and Knuth (1974)

Algorithm 1 (EFT of the sum of 2 floating point numbers with $|a| \geq |b|$)

function $[x, y]$ = `FastTwoSum`(a, b)
$x = \mathrm{fl}(a + b)$
$y = \mathrm{fl}((a - x) + b)$

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

function $[x, y]$ = `TwoSum`(a, b)
$x = \mathrm{fl}(a + b)$
$z = \mathrm{fl}(x - a)$
$y = \mathrm{fl}((a - (x - z)) + (b - z))$

EFT for the product (1/2)

$$x = \mathrm{fl}(a \cdot b) \quad \Rightarrow \quad a \cdot b = x + y \quad \text{with } y \in \mathbb{F},$$

Algorithm `TwoProduct` by Veltkamp and Dekker (1971)

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

Algorithm 3 (Error-free split of a floating point number into two parts)

function $[x, y] = \mathtt{Split}(a)$
  factor $= \mathrm{fl}(2^s + 1)$ % $\mathbf{u} = 2^{-p}$, $s = \lceil p/2 \rceil$
  $c = \mathrm{fl}(\mathtt{factor} \cdot a)$
  $x = \mathrm{fl}(c - (c - a))$
  $y = \mathrm{fl}(a - x)$

EFT for the product (2/2)

Algorithm 4 (EFT of the product of 2 floating point numbers)

function $[x, y] = \texttt{TwoProduct}(a, b)$
 $x = \mathrm{fl}(a \cdot b)$
 $[a_1, a_2] = \texttt{Split}(a)$
 $[b_1, b_2] = \texttt{Split}(b)$
 $y = \mathrm{fl}(a_2 \cdot b_2 - (((x - a_1 \cdot b_1) - a_2 \cdot b_1) - a_1 \cdot b_2))$

The Horner scheme

Algorithm 5 (Horner scheme)

function $\texttt{res} = \texttt{Horner}(p, x)$
  $s_n = a_n$
  for $i = n - 1 : -1 : 0$
    $p_i = \mathrm{fl}(s_{i+1} \cdot x)$ % rounding error π_i
    $s_i = \mathrm{fl}(p_i + a_i)$ % rounding error σ_i
  end
  $\texttt{res} = s_0$

$\gamma_n = n\mathbf{u}/(1 - n\mathbf{u}) \approx n\mathbf{u}$

$$\frac{|p(x) - \texttt{Horner}(p, x)|}{|p(x)|} \leq \underbrace{\gamma_{2n}}_{\approx 2n\mathbf{u}} \mathrm{cond}(p, x)$$

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

Algorithm 6 (Error-free transformation for the Horner scheme)

function $[\texttt{Horner}(p,x), p_\pi, p_\sigma] = \texttt{EFTHorner}(p,x)$
$s_n = a_n$
for $i = n-1 : -1 : 0$
  $[p_i, \pi_i] = \texttt{TwoProduct}(s_{i+1}, x)$
  $[s_i, \sigma_i] = \texttt{TwoSum}(p_i, a_i)$
  Let π_i be the coefficient of degree i of p_π
  Let σ_i be the coefficient of degree i of p_σ
end
$\texttt{Horner}(p,x) = s_0$

Compensated Horner scheme and its accuracy

Algorithm 7 (Compensated Horner scheme)

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

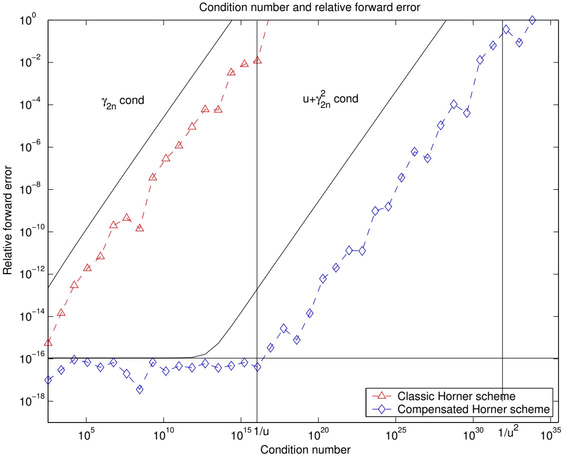
Theorem 1

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

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

Numerical experiments : testing the accuracy

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



Outline of the talk

Condition number for root finding

Definition 1

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

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

Theorem 2 (Chaitin-Chatelin and Frayssé)

Let p be a polynomial of degree n and x be a simple zero of p. The condition number of x is given by

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

Classic Newton's method

Algorithm 8 (Classic Newton's method)

$x_0 = \xi$

$x_{i+1} = x_i - \frac{p(x_i)}{p'(x_i)}$

$$\frac{|x_{i+1} - x|}{|x|} \approx \gamma_{2n}\,\mathrm{cond}(p, x)$$

Accurate Newton's method

Algorithm 9 (Accurate Newton's method)

$x_0 = \xi$

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

Using a theorem of Tisseur[1], one can show

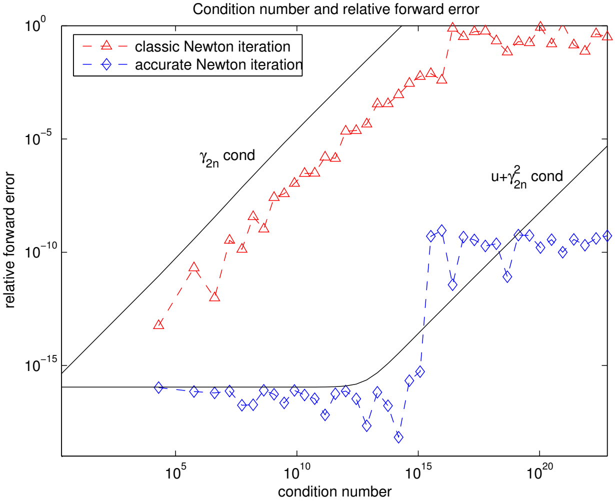
Theorem 3

Assume that there is an x such that $p(x) = 0$ and $p'(x) \neq 0$ is not too small. Assume also that $\mathbf{u} \cdot \mathrm{cond}(p, x) \leq 1/8$ for all i.
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

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

[1] Newton's Method in Floating Point Arithmetic and Iterative Refinement of Generalized Eigenvalue Problems, *SIAM J. Matrix Anal. Appl.*, 22(4) : 1038-1057, 2001

Numerical experiments



Accuracy of the classic Newton iteration and of the accurate Newton iteration

Conclusion

- Deal with zeros with multiplicities *via* an accurate modified Newton's method
- Use of deflation to also deal with multiplicities

Thank you for your attention