Analyse d'Algorithmes en Arithmétique à Virgule Flottante

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Context

Starting point:

How do numerical algorithms behave in finite precision arithmetic?

Typically,

- basic matrix computations: $Ax = b$, ...
- floating-point data and arithmetic as specified by IEEE 754.

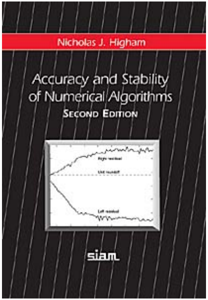
Ideally, we'd like to guarantee a priori that the computed solution $\widehat{x}$ has some kind of numerical quality:

- the forward error $\|x - \widehat{x}\|$ is 'small',
- the backward error $\|\Delta A\|$ such that $(A + \Delta A)\widehat{x} = b$ is 'small'.

Context

To get such guarantees, a key tool is backward error analysis:

- developed by Wilkinson in the 1960's,
- identifies nearby problems solved exactly: $\widehat{x} = (A + \Delta A)^{-1} b$,
- relies on a standard model of floating-point arithmetic,
- eminently powerful; see e.g. Higham's book:



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The standard model says that the result $\widehat{r}$ of a single operation $x \,\mathrm{op}\, y$ in floating-point arithmetic satisfies

$$\widehat{r} = (x \,\mathrm{op}\, y) \times (1 + \delta), \qquad |\delta| \leqslant u.$$

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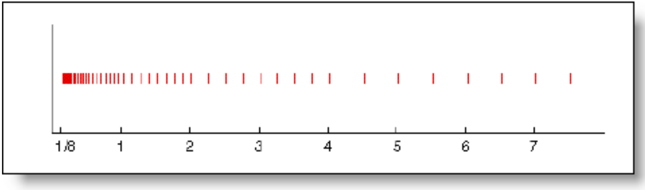
Our goal: show the benefits of exploiting some lower-level features:

1. Optimal bounds for basic operations,
2. Simpler and sharper Wilkinson-style error analysis,
3. Explain why some tiny kernels behave so well.

Floating-point data

$$\mathbb{F} := \{0\} \cup \left\{ \pm M \cdot \beta^{e-p+1} \;:\; \beta^{p-1} \leqslant M < \beta^{p},\;\; e_{\min} \leqslant e \leqslant e_{\max} \right\}.$$

- base β,
- precision p,
- exponent range defined by $e_{\min}$ and $e_{\max}$.



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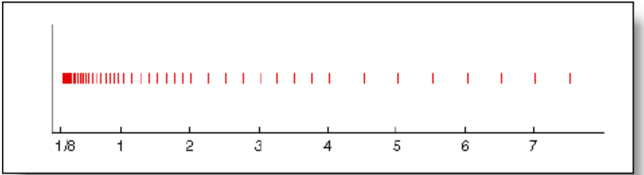

We assume

- $e_{\min} = -\infty$ and $e_{\max} = +\infty$: unbounded exponent range,
- β is even.

Floating-point data

- $x \in \mathbb{F} \backslash \{0\} \quad \Rightarrow \quad |x| = m \cdot \beta^e, \quad m = (*.\underbrace{* \cdots *}_{p-1})_\beta \in [1, \beta).$

- Three useful "units":
  - Unit in the first place: $\mathrm{ufp}(x) = \beta^e$,
  - Unit in the last place: $\mathrm{ulp}(x) = \beta^{e-p+1}$,
  - Unit roundoff: $u = \frac{1}{2}\beta^{1-p}$.

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- Alternative views, which display the structure of $\mathbb{F}$ very well:
  - $x \in \mathrm{ulp}(x)\mathbb{Z}$,
  - $|x| = (1 + 2ku)\,\mathrm{ufp}(x), \quad k \in \mathbb{N}$.

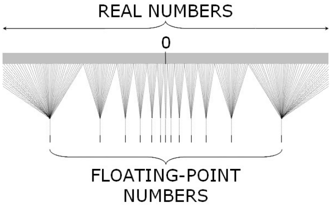
$$\Rightarrow \quad \mathbb{F} \cap [1, \beta) = \Big\{1, 1+2u, 1+4u, \dots\Big\}.$$

Rounding function

Round-to-nearest function $\mathrm{RN} : \mathbb{R} \to \mathbb{F}$ such that

$$\forall t \in \mathbb{R}, \qquad |\mathrm{RN}(t) - t| = \min_{f \in \mathbb{F}} |f - t|,$$

with given tie-breaking rule.



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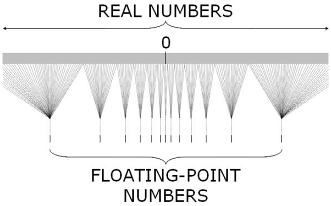

- $t \in \mathbb{F} \;\Rightarrow\; \mathrm{RN}(t) = t$
- RN nondecreasing
- reasonable tie-breaking rule:
  - $\mathrm{RN}(-t) = -\mathrm{RN}(t)$
  - $\mathrm{RN}(t\beta^e) = \mathrm{RN}(t)\beta^e, \; e \in \mathbb{Z}$

Error bounds for real numbers

$$E_1(t) := \frac{|\mathrm{RN}(t) - t|}{|t|} \leqslant \frac{u}{1+u}, \qquad E_2(t) := \frac{|\mathrm{RN}(t) - t|}{|\mathrm{RN}(t)|} \leqslant u.$$

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Bound $\frac{u}{1+u}$: sharp and well known [Dekker'71, Holm'80, Knuth'81-98], but simpler bound u almost always used in practice.

Correct rounding

This is the result of the composition of two functions: basic operations performed exactly, and exact result then rounded:

$$x, y \in \mathbb{F}, \quad \mathrm{op} = \pm, \times, \div \qquad \Rightarrow \qquad \text{return } \widehat{r} := \mathrm{RN}(x \,\mathrm{op}\, y).$$

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- The error bounds on E_1 and E_2 yield two standard models:

$$\begin{aligned} \widehat{r} &= (x \,\mathrm{op}\, y) \times (1 + \delta_1), \qquad && |\delta_1| \leqslant \tfrac{u}{1+u} =: u_1, \\ &= (x \,\mathrm{op}\, y) \times \frac{1}{1 + \delta_2}, && |\delta_2| \leqslant u. \end{aligned}$$

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- High relative accuracy is ensured:

$$\begin{aligned}
\widehat{r} &= \frac{\mathrm{RN}(x+y)}{2}(1+\delta_1), \qquad |\delta_1| \leqslant u_1, \\
&= \frac{x+y}{2}(1+\delta_1)(1+\delta_1'), \qquad |\delta_1'| \leqslant u_1, \\
&=: r\,(1+\epsilon), \qquad |\epsilon| \leqslant 2u.
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- We'd also like to have $\min(x,y) \leqslant \widehat{r} \leqslant \max(x,y)$ ...

Example

✗ Not always true:

$$\beta = 10,\ \ p = 3 \quad \Rightarrow \quad \mathrm{RN}\left(\frac{\mathrm{RN}\big(5.01 + 5.03\big)}{2}\right) = \mathrm{RN}\left(\frac{10}{2}\right) = 5.$$

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Proof for base two:

- $\widehat{r} := \mathrm{RN}\left(\frac{\mathrm{RN}(x+y)}{2}\right) = \mathrm{RN}\left(\frac{x+y}{2}\right)$.
- $x \leqslant \frac{x+y}{2} \leqslant y \quad \Rightarrow \quad \mathrm{RN}(x) \leqslant \mathrm{RN}\left(\frac{x+y}{2}\right) \leqslant \mathrm{RN}(y)$

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  $\Rightarrow \quad x \leqslant \widehat{r} \leqslant y.$ □

$\hookrightarrow$ Repair other cases using $r = x + \frac{y-x}{2}$. [Sterbenz'74, Boldo'15]

Conditions for exact subtraction

Sterbenz' lemma: [Sterbenz'74]

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- Proof: [Hauser'96]
  - assume $0 < y \leqslant x \leqslant 2y$.
  - $\mathrm{ulp}(y) \leqslant \mathrm{ulp}(x) \ \Rightarrow \ x - y \in \beta^e\mathbb{Z}$ with $\beta^e = \mathrm{ulp}(y)$.
  - $\frac{x-y}{\beta^e}$ is an integer such that $0 \leqslant \frac{x-y}{\beta^e} \leqslant \frac{y}{\mathrm{ulp}(y)} < \beta^p$. $\square$

Representable error terms

Addition and multiplication:

$$x, y \in \mathbb{F}, \quad \mathrm{op} \in \{+, \times\} \qquad \Rightarrow \qquad x \,\mathrm{op}\, y - \mathrm{RN}(x \,\mathrm{op}\, y) \in \mathbb{F}.$$

Division and square root:

$$x - y\,\mathrm{RN}(x/y) \in \mathbb{F}, \qquad x - \mathrm{RN}\left(\sqrt{x}\right)^2 \in \mathbb{F}.$$

- Noted quite early. [Dekker'71, Pichat'76, Bohlender et al.'91]
- RN required only for ADD and SQRT. [Boldo & Daumas'03]

FMA: its error is the sum of *two* floats. [Boldo & Muller'11]

Error-free transformations (EFT)

Floating-point algorithms for computing such error terms exactly:

- $x + y - \mathrm{RN}(x + y)$ in 6 additions [Møller'65, Knuth] and not less [Kornerup, Lefèvre, Louvet, Muller'12]

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  - in 17 + and x [Dekker'71, Boldo'06]
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- Similar FMA-based EFT for DIV, SQRT ... and FMA.

EFT are key for extended precision algorithms: *error compensation* [Kahan'65, ..., Higham'96, Ogita, Rump, Oishi'04+, Graillat, Langlois, Louvet'05+, ...], *floating-point expansions* [Priest'91, Shewchuk'97, Joldes, Muller, Popescu'14+].

Optimal relative error bounds

When t can be any real number, $E_1(t) \leqslant \frac{u}{1+u}$ and $E_2(t) \leqslant u$ are best possible:

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These are examples of **optimal bounds**:

- valid for all (t, RN) with t of a certain type;
- attained for some (t, RN) with t parametrized by β and p.

Can we do better when $t = x\,\mathbf{op}\,y$ and $x, y \in \mathbb{F}$?

This depends on *op* and, sometimes, on β and p. [J. & Rump'14]

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t	optimal bound on $E_1(t)$	optimal bound on $E_2(t)$
$x \pm y$	$\frac{u}{1+u}$	u
xy	$\frac{u}{1+u}$ $(\star)$	u $(\star)$
x/y	$\begin{cases} \frac{u}{1+u} & \text{if } \beta > 2, \\ u - 2u^2 & \text{if } \beta = 2 \end{cases}$	$\begin{cases} u & \text{if } \beta > 2, \\ \frac{u-2u^2}{1+u-2u^2} & \text{if } \beta = 2 \end{cases}$
$\sqrt{x}$	$1 - \frac{1}{\sqrt{1+2u}}$	$\sqrt{1+2u} - 1$

$(\star)$ iff $\beta > 2$ or $2^p + 1$ is not a Fermat prime.

$\longrightarrow$ **Two standard models for *each* arithmetic operation.**
$\longrightarrow$ **Application: sharper bounds and/or much simpler proofs.**

Context

Floating-point arithmetic

Error properties of arithmetic operations over $\mathbb{F}$

Some Wilkinson's bounds made simpler and sharper

Analyzing highly accurate kernels

Conclusion

Floating-point summation

Given $x_1, \ldots, x_n \in \mathbb{F}$, evaluate their sum in any order.

Classical analysis [Wilkinson'60]:

- Apply the standard model $n-1$ times.
- Deduce that the computed value $\widehat{s} \in \mathbb{F}$ satisfies

$$\left|\widehat{s} - \sum_{i=1}^{n} x_i\right| \leqslant \alpha \sum_{i=1}^{n} |x_i|, \qquad \alpha = (1+u)^{n-1} - 1.$$

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$$\frac{\text{error}}{\text{error bound}} \to 1 \text{ as } u \to 0.$$

✗ But $\alpha = (n-1)u + O(u^2)$, which hides a constant.
So, classically bounded as

$$\alpha \leqslant \gamma_{n-1}, \qquad \gamma_k = \frac{ku}{1-ku}, \qquad ku < 1.$$

[Higham'96]

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To prove this,

✗ don't use just the *refined* standard model, since

$$(1 + \tfrac{u}{1+u})^{n-1} - 1 \leqslant (n-1)u$$

only for $n \leqslant 4$.

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- $\widehat{s} = \sum_i x_i(1+\theta_i)$,
- $|\widehat{s} - \sum_i x_i| \leqslant \max_i |\theta_i| \cdot \sum_i |x_i|$,

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since for

$$1 + u - u + u - u + \cdots$$

and RN with ties 'to away'

$$\max_i |\theta_i| = (1 + \tfrac{u}{1+u})^{n-1} - 1$$
$$= (n-1)u + O(u^2).$$

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To prove this,

- Proceed *forward*;
- Combine

$$|\mathrm{RN}(x+y) - (x+y)| \leqslant \tfrac{u}{1+u}|x+y|, \tag{1}$$

with the lower-level property

$$\begin{aligned} |\mathrm{RN}(x+y) - (x+y)| &\leqslant |f - (x+y)|, \qquad \forall f \in \mathbb{F}, \\ &\leqslant \min\{|x|, |y|\}; \end{aligned} \tag{2}$$

A simpler, $O(u^2)$-free bound

Theorem [Rump'12]

For recursive summation, one can take $\alpha = (n-1)u$.

To prove this,

- Proceed *forward*;
- Combine

$$|\mathrm{RN}(x+y) - (x+y)| \leqslant \tfrac{u}{1+u}|x+y|, \tag{1}$$

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- Conclude by induction on n with a clever case-distinction comparing $|x_n|$ to $u \cdot \sum_{i<n} |x_i|$, and using either (1) or (2).

Wilkinson's bounds revisited

Problem	Classical α	New α	Ref.
summation	$(n-1)u + O(u^2)$	$(n-1)u$	[1]

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summation	$(n-1)u + O(u^2)$	$(n-1)u$		[1]
dot prod., mat. mul.	$nu + O(u^2)$	nu		[1]
Euclidean norm	$(\frac{n}{2}+1)u + O(u^2)$	$(\frac{n}{2}+1)u$		[2]
$Tx = b, \quad A = LU$	$nu + O(u^2)$	nu		[2]
$A = R^T R$	$(n+1)u + O(u^2)$	$(n+1)u$		[2]
x^n (recursive, $\beta = 2$)	$(n-1)u + O(u^2)$	$(n-1)u$	$(\star)$	[3]
product $x_1 x_2 \cdots x_n$	$(n-1)u + O(u^2)$	$(n-1)u$	$(\star)$	[4]
poly. eval. (Horner)	$2nu + O(u^2)$	$2nu$	$(\star)$	[4]

$(\star)$ if $n < O(1/\sqrt{u})$

[1]: with Rump'13; [2]: with Rump'14; [3]: Graillat, Lefèvre, Muller'14;
[4]: with Bünger and Rump'14.

Remarks

- Except for Horner's rule, these bounds hold for any ordering.
- Further refinements are possible:
  - using $u_1 := \frac{u}{1+u}$ instead of u;
  - assuming recursive summation and $20nu < 1$. [Mascarenhas'16]

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- Except for Horner's rule, these bounds hold for any ordering.
- Further refinements are possible:
  - using $u_1 := \frac{u}{1+u}$ instead of u;
  - assuming recursive summation and $20nu < 1$. [Mascarenhas'16]
- Key ingredients for analyzing Horner's rule in degree n:
  - see it as $(\times)(+\times)\cdots(+\times)(+)$;
  - bound the relative error of $\mathrm{RN}\big(\mathrm{RN}(x+y)z\big)$ by

$$(1+u_1)(1+u_\varphi)-1, \qquad u_\varphi \approx \frac{u}{1+\sqrt{u}};$$

  - show that $\alpha \leqslant (1+u_1)^{n+1}(1+u_\varphi)^{n-1} - 1 \leqslant 2nu$.

Kahan's algorithm for $ad - bc$

Kahan's algorithm uses the FMA to evaluate $\det \begin{bmatrix} a & b \\ c & d \end{bmatrix} = ad - bc$:

$$\boxed{\begin{array}{l} \widehat{w} := \mathrm{RN}(bc); \\ \widehat{f} := \mathrm{RN}(ad - \widehat{w}); \quad e := \mathrm{RN}(\widehat{w} - bc); \\ \widehat{r} := \mathrm{RN}(\widehat{f} + e); \end{array}}$$

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- The operation $ad - bc$ is not in IEEE 754, but very common:
  - complex arithmetic,
  - discriminant of a quadratic equation,
  - robust orientation predicates using tests like '$ad - bc > \epsilon$?'
- If evaluated naively, $ad - bc$ leads to highly inaccurate results:

$$\frac{|\widehat{f} - r|}{|r|} \text{ can be of the order of } u^{-1} \gg 1.$$

Kahan's algorithm for $ad - bc$

- Analysis in the standard model [Higham'96]:

$$\frac{|\widehat{r} - r|}{|r|} \leqslant 2u \left(1 + \frac{u|bc|}{2|r|}\right).$$

$\Rightarrow$ high relative accuracy **as long as** $u|bc| \not\gg 2|r|$.

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In fact, Kahan's algorithm is **always** highly accurate:

✗ the standard model alone fails to predict this;

✗ misinterpreting bounds $\Rightarrow$ dismissing good algorithms.

Further analysis

[J., Louvet, Muller'13]

The key is an ulp-analysis of the error terms ϵ_1 and ϵ_2 given by:

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- Since e is exactly $\widehat{w} - bc$, we have $\widehat{r} - r = \epsilon_1 + \epsilon_2$.
- Furthermore, we can prove that $|\epsilon_i| \leqslant \frac{\beta}{2}\mathrm{ulp}(r)$ for $i = 1, 2$.

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These bounds mean Kahan's algorithm is **always** highly accurate.

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We can do better via a case analysis comparing $|\epsilon_2|$ to $\frac{1}{2}\text{ulp}(r)$:

Theorem:

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Theorem:

- relative error $|\widehat{r} - r|/|r| \leqslant 2u$;
- this bound is asymptotically optimal.

Certificate of optimality

This is an explicit input set parametrized by β and p such that

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Example: for Kahan's algorithm for $r = ad - bc$:

$$\left.\begin{aligned} a &= b = \beta^{p-1} + 1 \\ c &= \beta^{p-1} + \tfrac{\beta}{2}\beta^{p-2} \\ d &= 2\beta^{p-1} + \tfrac{\beta}{2}\beta^{p-2} \end{aligned}\right\} \quad \Rightarrow \quad \frac{|\widehat{r} - r|/|r|}{2u} = \frac{1}{1 + \beta^{1-p}} = 1 - 2u + O(u^2).$$

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- Optimality is asymptotic, but often OK in practice: for $\beta = 2$ and $p = 11$, the above example has relative error $1.999024\ldots u$.
- The certificate consists of sparse, symbolic floating-point data, which we can handle automatically. [J., Louvet, Muller, Plet]

Summary

Floating-point arithmetic is

- specified rigorously by IEEE 754,
- highly structured and much richer than the standard model.

Exploiting this structure leads to

- optimal standard models for basic arithmetic operations,
- simpler and sharper Wilkinson-like bounds,
- proofs of nice behavior of some numerical kernels.

Future directions

Optimal error bounds for complex arithmetic:

- Naive evaluation of $z = (a + ib)(c + id)$ in floating-point
  $\Rightarrow \quad |\widehat{z} - z|/|z| \leqslant \sqrt{5}\, u$ [Brent, Percival, Zimmermann'07]
- Similar results for other schemes [with Kornerup, Louvet, Muller'14]
- For inversion, best constant ≈ 2.7 [with Louvet, Muller, Plet'15]
- Best constants for division and square root?

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Robustness issues

- What if roundings other than *to nearest*? [Demmel, Nguyen'13], [Boldo, Graillat, Muller'16]; [Ozaki, Ogita, Bünger, Oishi'15]
- How to take underflow and overflow into account?