Probabilistic rounding error analysis for large scale, low precision scientific computing

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lecture based on joint work with Nick Higham (Univ. Manchester)

AFAE course, Sorbonne Université (2019 version)

An example: recursive summation

Let $s = \sum_{i=1}^{n} x_i$ be computed by recursive summation:

$s_1 = x_1$ for $i = 2$ to n $\quad s_i = s_{i-1} + x_i$ end $(s = s_n)$	$s_1 = x_1$ for $i = 2$ to n $\quad \widehat{s}_i = (\widehat{s}_{i-1} + x_i)(1 + \delta_i), \quad \lvert\delta_i\rvert \le u$ end $(\widehat{s} = \widehat{s}_n)$

We have the bound

$$\frac{|\widehat{s} - s|}{|s|} \le (n-1)\kappa u + O(u^2), \qquad \kappa = \frac{\sum_{i=1}^{n} |x_i|}{\left|\sum_{i=1}^{n} x_i\right|}$$

- Many efforts focus on getting small error even for large κ
- What about n?

Historical perspective

- Backward error analysis was developed by James Wilkison in the 1960s
- At that time, $n = 100$ was huge! Solving linear systems of $n = O(10)$ equations would take days

$\Rightarrow$ n was considered a "constant"

Hence traditional error analysis has paid little attention to n

> *The **constant** terms in an error bound are the least important parts of error analysis. It is not worth spending much effort to minimize constants because the achievable improvements are usually insignificant.*
>
> *Nick Higham, ASNA 2ed (2002)*

Today: large scale problems

- Since the 1990s, the TOP500 list ranks the world's most powerful supercomputers based on their ability to solve linear systems of equations $Ax = b$ as fast as possible

The Summit supercomputer

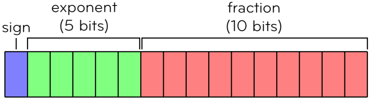
- In the latest ranking (Nov. 2019), the #1 computer solved a linear system of 16 million equations in 5.5 hours

Today: low precision arithmetics

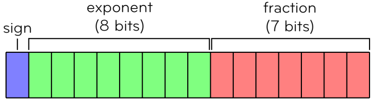
Type		Bits	Range	$u = 2^{-t}$
fp64	double	64	$10^{\pm 308}$	$2^{-53} \approx 1 \times 10^{-16}$
fp32	single	32	$10^{\pm 38}$	$2^{-24} \approx 6 \times 10^{-8}$
fp16	half	16	$10^{\pm 5}$	$2^{-11} \approx 5 \times 10^{-4}$
bfloat16	half	16	$10^{\pm 38}$	$2^{-8} \approx 4 \times 10^{-3}$

Half precision increasingly **supported by hardware**:

- Present: **NVIDIA** Pascal & Volta GPUs, **AMD** Radeon Instinct MI25 GPU, **Google** TPU, **ARM** NEON
- Near future: Fujitsu A64FX ARM, **IBM** AI chips, **Intel** Xeon Cooper Lake and Intel Nervana Neural Network

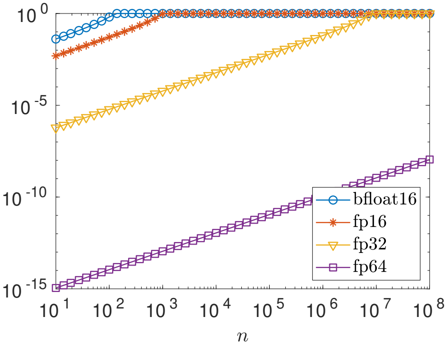


fp16



bfloat16

Backward stability guarantees are lost



In half precision, backward error of order 1 for $n > 1024$ (fp16) or $n > 128$ (bfloat16)

Not a single correct digit guaranteed when n and/or u are large, even if $\kappa = 1$!

For large scale and/or low precision computations, **bounds of the form *nu* are no longer acceptable**

A first summation error analysis

Recursive summation computes

$$\widehat{s}_i = (\widehat{s}_{i-1} + x_i)(1+\delta_i), \quad i = 2\colon n \qquad \text{with } \widehat{s}_1 = s_1 = x_1$$

$$\begin{aligned}
\widehat{s} - s = \widehat{s}_n - s_n &= \widehat{s}_{n-1} - s_{n-1} + (\widehat{s}_{n-1} + x_n)\delta_n \\
&= \sum_{i=2}^{n} (\widehat{s}_{i-1} + x_i)\delta_i = \sum_{i=2}^{n} \widehat{s}_i \delta_i/(1+\delta_i) = \sum_{i=2}^{n} s_i\delta_i + O(u^2)
\end{aligned}$$

First-order worst-case bound:

$$|\widehat{s} - s| \le \sum_{i=2}^{n} |s_i||\delta_i| \le \sum_{i=2}^{n}\sum_{j=1}^{i} |x_j|\, u \le (n-1)\sum_{j=1}^{n} |x_j|\, u$$

This bound is however attained only when

$$\forall i \ \delta_i = +u \text{ or } \forall i \ \delta_i = -u$$

$\Rightarrow$ intuitively seems very unlikely!

Modelling rounding errors as random variables

Since the 1960s, researchers have tried modelling the δ_i as independent random variables to translate the intuition that they are probably not all equal to $+u$ or $-u$

It is important to realize that rounding errors are **not** random:

- For a given input, order of computation, and deterministic rouding mode, rounding errors are entirely predetermined
- Successive δ_i are dependent:

$$\begin{aligned} \mathrm{fl}\big((a+b)+c\big) &= \mathrm{fl}\big(\mathrm{fl}(a+b)+c\big) = \mathrm{fl}\big((a+b)(1+\delta_1)+c\big) \\ &= \big((a+b)(1+\delta_1)+c\big)(1+\delta_2) \end{aligned}$$

> *There is no claim that ordinary rounding and chopping are random processes, or that successive errors are independent.* ***The question to be decided is whether or not these particular probabilistic models of the processes will adequately describe what actually happens.***
>
> *— Hull and Swenson, 1966*

A first basic probabilistic analysis

- Assume δ_i are independent random variables uniformly distributed on $[-u, +u]$
- Law of large numbers: $\widehat{s} - s = \sum_{i=2}^{n} s_i \delta_i$ converges towards $\mathbb{E}(\widehat{s} - s) = \sum_{i=2}^{n} s_i \, \mathbb{E}(\delta_i) = 0$ when $n \to \infty$

Central limit theorem (classical variant)

Let X_1, ..., X_n i.i.d. random variables of mean μ and variance σ^2, and let $S_n = \frac{1}{n} \sum_{i=1}^{n} X_i$. For large enough n, $\sqrt{n}(S_n - \mu)$ follows the normal distribution $\mathcal{N}(0, \sigma^2)$.

- For $X_i \leftarrow \delta_i$, $\mu = 0$ and $\sigma^2 = u^2/3 \Rightarrow \frac{\sum_{i=1}^{n} \delta_i}{\sqrt{n-1}} \sim \mathcal{N}(0, u^2/3)$
- Problem: $X_i \leftarrow s_i \delta_i$ are **not** identically distributed

Central limit theorem (Lyapunov's variant)

Let X_1, ..., X_n independent random variables of mean μ_i and variance σ_i^2. Let $\mathfrak{S}_n^2 = \sum_{i=1}^n \sigma_i^2$ and let $S_n = \sum_{i=1}^n X_i - \mu_i$. For large enough n, and under Lyapunov's condition, $S_n/\mathfrak{S}_n$ follows the normal distribution $\mathcal{N}(0,1)$.

Lyapunov's condition: for some $\epsilon > 0$,

$$\lim_{n\to\infty} \frac{1}{\mathfrak{S}_n^{2+\epsilon}} \sum_{i=1}^{n} \mathbb{E}\left(|X_i - \mu_i|^{2+\epsilon}\right) = 0$$

For $X_i \leftarrow s_i\delta_i$, $\mathfrak{S}_{n-1}^2 = \sum_{i=2}^n s_i^2\, u^2/3$ and so

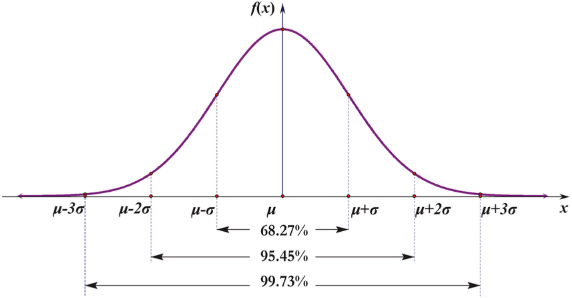
$$\mathfrak{S}_{n-1} \leq \sqrt{(n-1)/3} \sum_{j=1}^{n} |x_j|\, u$$

The 3σ rule

For a random variable $X \sim \mathcal{N}(\mu, \sigma^2)$, the probability that $X \in [\mu - \lambda\sigma, \mu + \lambda\sigma]$ is given by $\Phi(\lambda) - \Phi(-\lambda)$ where

$$\Phi(\lambda) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\lambda} e^{-t^2/2} dt$$

In particular, $\Phi(3) - \Phi(-3) \approx 99.7\%$.



- $(\widehat{s} - s)/\mathfrak{S}_{n-1} \sim \mathcal{N}(0, 1)$ and so we have with 99.7% probability

$$|\widehat{s} - s| \leq 3\mathfrak{S}_{n-1} \leq \sqrt{3(n-1)} \sum_{j=1}^{n} |x_j|\, u + O(u^2)$$

Wilkinson's rule of thumb

In general, the statistical distribution of the rounding errors will reduce considerably the function of n occurring in the relative errors. We might expect in each case that this function should be replaced by something which is no bigger than its square root.

— James Wilkinson, 1961

Why is it a **"rule of thumb"**?

- Assumptions on δ_i: which are really needed? Which are true in practice?
- Use of central limit theorem requires $n \to \infty$
- Since $X_i = s_i\delta_i$ are not identically distributed Lyapunov's condition must also hold
- Only a first order bound
- Only for summation? Does it generalize to other algorithms?

A more general probabilistic model

We will show that the assumptions made by the following more general model are sufficient to obtain a $O(\sqrt{n}u)$ bound

Probabilistic model of rounding errors

In the computation of interest, the quantities δ in the model

$$\mathrm{fl}(a \text{ op } b) = (a \text{ op } b)(1+\delta), \quad |\delta| \le u, \quad \text{op} \in \{+,-,\times,\div\}$$

associated with every pair of operands are independent random variables of mean zero.

- No specific distribution (e.g., uniform) assumed
- Not necessarily identically distributed

Questions left for later:

- Are these assumptions as general as possible? (i.e., are they necessary? spoiler: no they're not)
- Are these assumptions satisfied in practice? (i.e., are they reasonable? spoiler: not always, but...)

Concentration inequalities

Central limit theorem is only valid asymptotically (for $n \to \infty$).
To obtain a rigorous result for a given n, we use the following concentration inequality

Hoeffding's inequality

Let X_1, ..., X_n be random independent variables satisfying $|X_i| \leq c$.
Then the sum $S = \sum_{i=1}^{n} X_i$ satisfies

$$\Pr(|S - \mathbb{E}(S)| \geq \lambda\sqrt{n}c) \leq 2\exp(-\lambda^2/2)$$

Two key assumptions:

- Independence $\to$ OK with our probabilistic model
- Boundedness $\to$ OK with standard FP model $|\delta_i| \leq u$

Resulting bound for summation

Recall that $\widehat{s} - s = \sum_{i=2}^{n} s_i \delta_i$
Exercise: apply Hoeffding's inequality to $X_i \leftarrow s_i \delta_i$

Resulting bound for summation

Recall that $\widehat{s} - s = \sum_{i=2}^{n} s_i \delta_i$

Exercise: apply Hoeffding's inequality to $X_i \leftarrow s_i \delta_i$

- Independence $\rightarrow$ OK because independence of δ_i
- Boundedness $\rightarrow$ OK $|X_i| \leq c_i = \sum_{j=1}^{i} |x_j|\, u$

Apply Hoeffding's inequality to $S = \sum_{i=2}^{n} X_i$ with
$c = \max c_i = \sum_{j=1}^{n} |x_j|\, u$ to obtain with probability $\exp(-\lambda^2/2)$

$$|S - \mathbb{E}(S)| = |S| = |\widehat{s} - s| \leq \lambda \sqrt{n-1} \sum_{j=1}^{n} |x_j|\, u$$

This bound is for summation only... what about inner products? matrix–matrix multiplication? solution to linear systems? eigenvalue decompositions? polynomial computations? etc. etc.

Systematizing the analysis: backward error analysis

$$\widehat{s}_2 = (x_1 + x_2)(1 + \delta_2)$$
$$\widehat{s}_k = (\widehat{s}_{k-1} + x_k)(1 + \delta_k) = x_1 \prod_{j=2}^{k} (1 + \delta_j) + \ldots + x_k(1 + \delta_k)$$
$$\widehat{s}_n = \widehat{s} = \sum_{i=1}^{n} x_i \prod_{j=\max(i,2)}^{n} (1 + \delta_j), \qquad |\delta_j| \le u$$

Fundamental lemma in backward error analysis

If $|\delta_i| \le u$ for $i = 1 : n$ and $nu < 1$, then
$$\prod_{i=1}^{n} (1 + \delta_i) = 1 + \theta_n, \quad |\theta_n| \le \gamma_n := \frac{nu}{1 - nu} = nu + O(u^2)$$

This fundamental lemma can be applied to essentially any numerical algorithm $\Rightarrow$ can we obtain an analogous probabilistic lemma?

Probabilistic backward error analysis

- Main difficulty: $\prod_{i=1}^{n}(1+\delta_i)$ is a product, but probabilistic tools (CLT, concentration ineq) apply to sums

- Transform the product in a sum by taking the logarithm

$$S = \log \prod_{i=1}^{n}(1+\delta_i) = \sum_{i=1}^{n} \log(1+\delta_i)$$

- Taylor: $\log(1+\delta_i) = \sum_{k=1}^{\infty} \frac{(-1)^{k+1}\delta_i^k}{k}$
  - $\log(1+\delta_i) \le \delta_i + \sum_{k=2}^{\infty} |\delta_i|^k = \delta_i + \frac{\delta_i^2}{1-|\delta_i|}$
  - $\log(1+\delta_i) \ge \delta_i - \sum_{k=2}^{\infty} |\delta_i|^k = \delta_i - \frac{\delta_i^2}{1-|\delta_i|}$

$\Rightarrow$ $|\log(1+\delta_i)| \le u + \frac{u^2}{1-u} = \frac{u}{1-u} := c$

Probabilistic backward error analysis (cont'd)

- **Exercise:** use Hoeffding's ineq to $X_i \leftarrow \log(1 + \delta_i)$ to bound $|S|$

Probabilistic backward error analysis (cont'd)

- **Exercise:** use Hoeffding's ineq to $X_i \leftarrow \log(1+\delta_i)$ to bound $|S|$

$$|S - \mathbb{E}(S)| \le \lambda\sqrt{n}c = \frac{\lambda\sqrt{n}u}{1-u}$$

with probability $\exp(-\lambda^2/2)$

  - $\mathbb{E}(S) = \sum_{i=1}^{n} \mathbb{E}(\log(1+\delta_i))$
  - $|\mathbb{E}(\log(1+\delta_i))| \le \frac{u^2}{1-u}$

$\Rightarrow$ $|\mathbb{E}(S)| \le \frac{nu^2}{1-u}$

$$|S| \le \frac{\lambda\sqrt{n}u + nu^2}{1-u}$$

- Retrieve the result by taking the exponential of S:

$$\prod_{i=1}^{n}(1+\delta_i) = 1+\theta_n, \quad |\theta_n| \le \exp\left(\frac{\lambda\sqrt{n}u + nu^2}{1-u}\right) - 1 := \widetilde{\gamma}_n(\lambda)$$

For $0 < t < 1$, $e^t \le 1 + t/(1-t)$ gives

$$\widetilde{\gamma}_n(\lambda) \le \lambda\sqrt{n}u + O(u^2)$$

Probabilistic backward error analysis: main result

Main result

Let δ_i, $i = 1 : n$, be independent random variables of mean zero such that $|\delta_i| \le u$. Then, for any constant $\lambda > 0$, the relation

$$\prod_{i=1}^{n}(1+\delta_i) = 1 + \theta_n, \quad |\theta_n| \le \widetilde{\gamma}_n(\lambda) := \exp\left(\frac{\lambda\sqrt{n}u + nu^2}{1-u}\right) - 1$$

$$\le \lambda\sqrt{n}u + O(u^2)$$

holds with probability $P(\lambda) = 1 - 2\exp(-\lambda^2/2)$

Key features:

- Exact bound, not first order (and $nu < 1$ not required)
- No "$n \to \infty$" assumption (CLT $\to$ Hoeffding's inequality)
- Small values of λ suffice: $P(1) \approx 0.73$, $P(5) \ge 1 - 10^{-5}$
- Can be applied **in a nearly systematic way:** $\gamma_n \to \widetilde{\gamma}_n(\lambda)$

Application to summation, inner products

$$\widehat{s} = \sum_{i=1}^{n} x_i \prod_{j=\max(i,2)}^{n} (1+\delta_j) = \sum_{i=1}^{n} x_i (1+\theta_i)$$

$$\forall i \le n,\ \Pr\big(|\theta_i| \le \widetilde{\gamma}_{n-\max(i,2)+1}(\lambda)\big) \ge 1 - 2\exp(-\lambda^2/2)$$

$$\Rightarrow \Pr\big(\forall i \le n,\ |\theta_i| \le \widetilde{\gamma}_{n-\max(i,2)+1}(\lambda)\big) \ge 1 - 2n\exp(-\lambda^2/2)$$

$$\Rightarrow \Pr\big(\forall i \le n,\ |\theta_i| \le \widetilde{\gamma}_{n-1}(\lambda)\big) \ge 1 - 2n\exp(-\lambda^2/2)$$

Similarly, if $s = x^T y = \sum_{i=1}^{n} x_i y_i$, then

$$\widehat{s} = \sum_{i=1}^{n} x_i y_i (1+\epsilon_i) \prod_{j=\max(i,2)}^{n} (1+\delta_j) = \sum_{i=1}^{n} x_i y_i (1+\theta_i)$$

where

$$\Pr\big(\forall i \le n,\ |\theta_i| \le \widetilde{\gamma}_{n}(\lambda)\big) \ge 1 - 2n\exp(-\lambda^2/2)$$

Componentwise expression:

$$\widehat{s} = (x+\Delta x)^T y = x^T (y + \Delta y), \qquad |\Delta x| \le \widetilde{\gamma}_n(\lambda), \quad |\Delta y| \le \widetilde{\gamma}_n(\lambda)$$

Application to numerical linear algebra

Similarly to summation, repeated application of our main result yields the following bounds with probability $1 - 2F\exp(-\lambda^2/2)$

Algorithm	Bound	F
Matrix–vector product $y = Av$, $A \in \mathbb{R}^{m\times n}$, $v \in \mathbb{R}^n$	$\widetilde{\gamma}_n(\lambda)$	mn
Matrix–matrix product $C = AB$, $A \in \mathbb{R}^{m\times n}$, $B \in \mathbb{R}^{n\times p}$	$\widetilde{\gamma}_n(\lambda)$	mnp
LU factorization $A = LU$, $A \in \mathbb{R}^{n\times n}$	$\widetilde{\gamma}_n(\lambda)$	$n^3/3 + n^2/2 + n/6$
Triangular system $Tx = b$, $T \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$	$\widetilde{\gamma}_n(\lambda)$	$n^2/2 + n/2$
Linear system $Ax = b$, $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$	$3\widetilde{\gamma}_n(\lambda) + 2\widetilde{\gamma}_n(\lambda)^2$	$n^3/3 + 3n^2/2 + 7n/6$
Cholesky factorization $A = LL^T$, $A \in \mathbb{R}^{n\times n}$	$\widetilde{\gamma}_{n+1}(\lambda)$	$n^3/6 + n^2/2 + n/3$

$\Rightarrow$ n (in $\widetilde{\gamma}_n(\lambda)$) is the maximal number of products of terms $(1+\delta_i)$

$\Rightarrow$ $2F$ (in the prob.) $\approx$ equals the flops required by the algorithm

Keeping the probabilities independent of n

- Let the probability of failure $P_F(\lambda, n) = 2n \exp(-\lambda^2/2)$

- $P_F(5, 10) \approx 0.00007$ ... but $P_F(5, 10^5) \approx 0.7$!

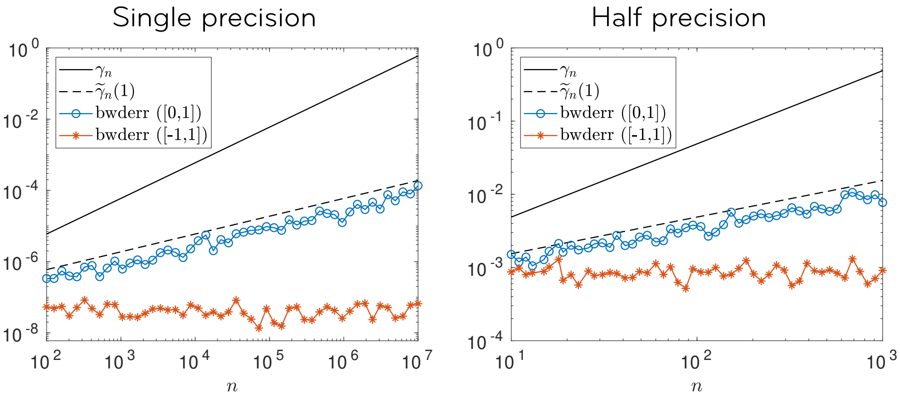
$\Rightarrow$ Crucial to keep the probabilities independent of n!
Fortunately:

$$P_F(\lambda, O(n^p)) = O(1) \quad \Leftrightarrow \quad \lambda = O(\sqrt{p \log n})$$

$\Rightarrow$ Error bound grows no faster than $\sqrt{n \log n}u$ for algorithms of polynomial complexity

- Moreover the constant hidden in the big O is small:
$$P_F(10, 10^{10}) \approx 4 \times 10^{-12}$$

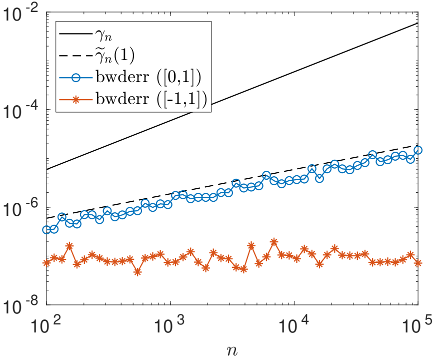
Numerical experiments with summation



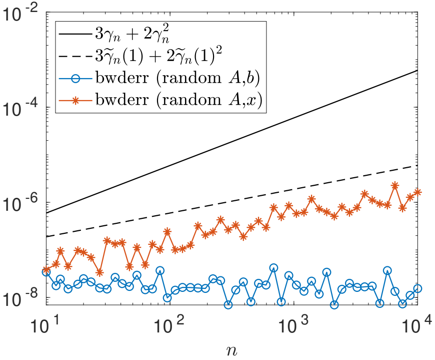
- Able to guarantee backward stability for a wider range of problems in a probabilistic sense
- $\widetilde{\gamma}_n$ is not always asymptotically sharp: error does not grow with n for $[-1, 1]$ data (we will come back to this observation later)

Experimental results with NLA algorithms

Matrix–vector product
(single precision)

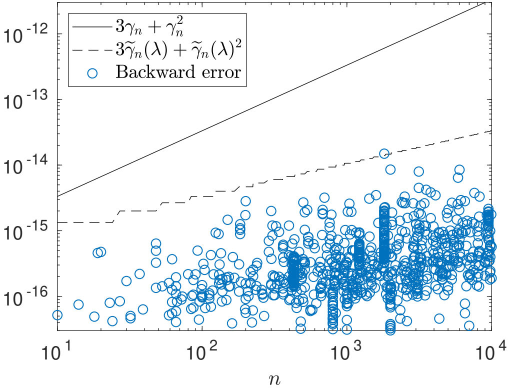


Solution to $Ax = b$
(single precision)



Experimental results with real-life matrices

Solution of $Ax = b$ (double precision),
for 943 matrices from the SuiteSparse collection



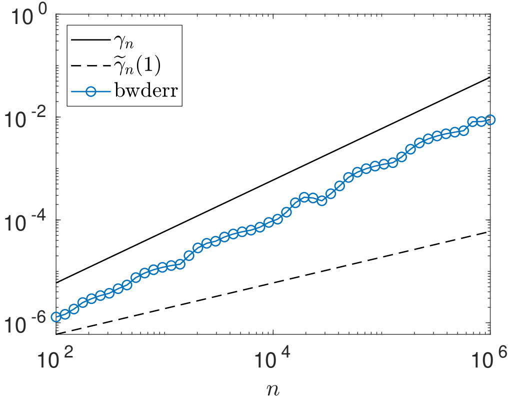
$\Rightarrow$ Probabilistic bound is thus satisfied in many important cases...
but there are counter-examples

Example with dependent rounding errors

Summation with constant x_i:

$$s_i = s_{i-1} + c, \qquad i = 2\colon n$$

leads to an error growing as nu rather than $\sqrt{n}u$

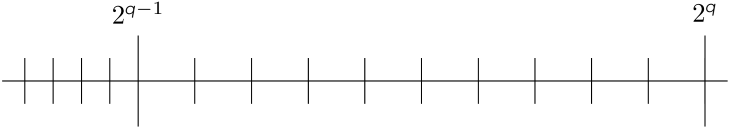


Exercise: explain what is happening

Example with dependent rounding errors (cont'd)

$$s_i = s_{i-1} + c \Rightarrow \quad \widehat{s}_i = (\widehat{s}_{i-1} + c)(1 + \delta_i)$$

Example with dependent rounding errors (cont'd)



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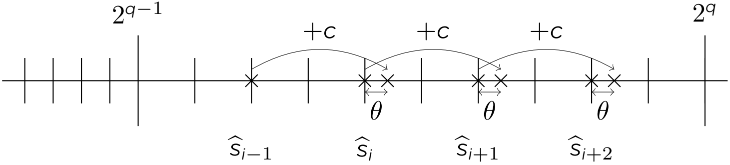
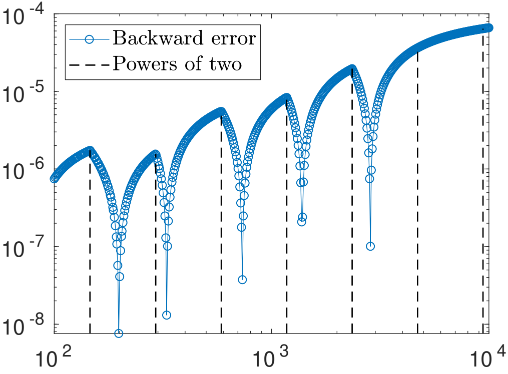
Example with dependent rounding errors (cont'd)



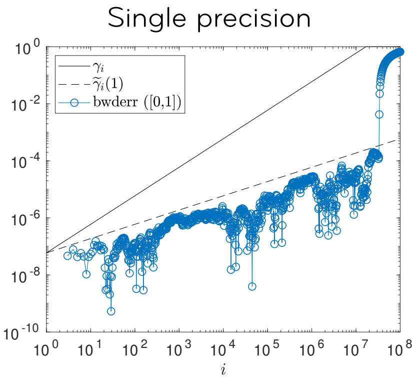
$$s_i = s_{i-1} + c \Rightarrow \quad \widehat{s}_i = (\widehat{s}_{i-1} + c)(1 + \delta_i)$$

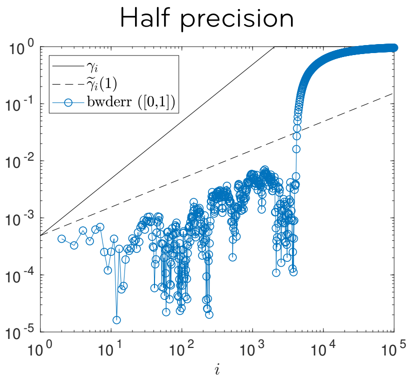
$\Rightarrow$ $\delta_i = \theta$ is constant within intervals $[2^{q-1}; 2^q]$



Example with rounding errors of nonzero mean

Summation of a very large number of nonnegative terms ($n \gg 10^3$ in half precision, $n \gg 10^7$ in single precision) leads to an error eventually growing like $O(nu)$





Exercise: explain what is happening

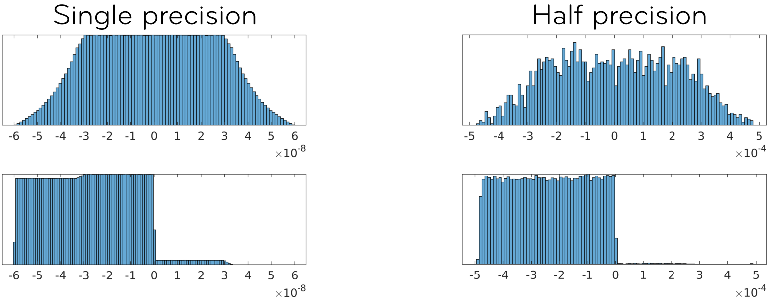
Example with rounding errors of nonzero mean (cont'd)

$$s_i = s_{i-1} + x_i \quad \Rightarrow \quad \widehat{s}_i = (\widehat{s}_{i-1} + x_i)(1 + \delta_i)$$

Example with rounding errors of nonzero mean (cont'd)

$$s_i = s_{i-1} + x_i \quad \Rightarrow \quad \widehat{s}_i = (\widehat{s}_{i-1} + x_i)(1 + \delta_i)$$

Distribution of the δ_i



Top: $1 \le i \le 3 \times 10^3$
Bottom: $3 \times 10^3 \le i \le 10^5$

Top: $1 \le i \le 3 \times 10^7$
Bottom: $3 \times 10^7 \le i \le 10^8$

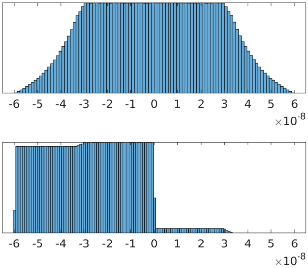
Example with rounding errors of nonzero mean (cont'd)

$$s_i = s_{i-1} + x_i \quad \Rightarrow \quad \widehat{s}_i = (\widehat{s}_{i-1} + x_i)(1+\delta_i)$$

Explanation: s_i keeps increasing, at some point, it becomes so large that $\widehat{s}_{i-1} \geq x_i/u$ and the computed sum **stagnates**: $\widehat{s}_i = \widehat{s}_{i-1}$.
Stagnation produces negative δ_i: indeed $\delta_i = -x_i/(\widehat{s}_{i-1} + x_i) < 0$

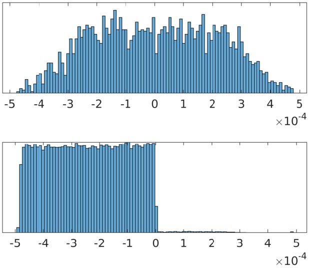
Distribution of the δ_i

Single precision



Top: $1 \leq i \leq 3 \times 10^3$
Bottom: $3 \times 10^3 \leq i \leq 10^5$

Half precision



Top: $1 \leq i \leq 3 \times 10^7$
Bottom: $3 \times 10^7 \leq i \leq 10^8$

Validity of the probabilistic bound

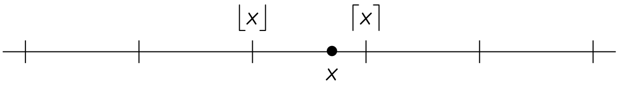
- The previous examples reveal situations in which the probabilistic bound is not valid, because the assumptions in the model are not satisfied

- Even though the analysis gives useful predictions, care is required in applying and interpreting the bound

... at least with a deterministic rounding mode such as **round to nearest** (which we have used so far)

⇒ what about **stochastic** rounding modes?

Stochastic rounding: definition



With round to nearest

$$\mathrm{fl}(x) = \begin{cases} \lceil x \rceil & \text{if } x - \lfloor x \rfloor > \lceil x \rceil - x \\ \lfloor x \rfloor & \text{otherwise} \end{cases}$$

Instead, with stochastic rounding

$$\mathrm{fl}(x) = \begin{cases} \lceil x \rceil & \text{with probability } p = \frac{x - \lfloor x \rfloor}{\lceil x \rceil - \lfloor x \rfloor} \\ \lfloor x \rfloor & \text{with probability } 1 - p = \frac{\lceil x \rceil - x}{\lceil x \rceil - \lfloor x \rfloor} \end{cases}$$

where $\lfloor \cdot \rfloor$ and $\lceil \cdot \rceil$ denote the operators that round down and up

Stochastic rounding $\Rightarrow$ zero mean δ_i

- Let $a, b \in \mathbb{R}$ and op $\in \{+, -, \times, \div\}$ such that

$$\mathrm{fl}(a \text{ op } b) = (a \text{ op } b)(1 + \delta)$$

- **Exercise:** prove that with stochastic rounding, $\mathbb{E}(\delta) = 0$

Stochastic rounding $\Rightarrow$ zero mean δ_i

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$$\mathrm{fl}(a \text{ op } b) = (a \text{ op } b)(1+\delta)$$

- **Exercise:** prove that with stochastic rounding, $\mathbb{E}(\delta) = 0$
- Let $x := a \text{ op } b$; with stochastic rounding,

$$\mathbb{E}(\mathrm{fl}(x)) = \frac{\lceil x \rceil \big(x - \lfloor x \rfloor\big) + \lfloor x \rfloor \big(\lceil x \rceil - x\big)}{\lceil x \rceil - \lfloor x \rfloor}$$

$$= \frac{x\big(\lceil x \rceil - \lfloor x \rfloor\big)}{\lceil x \rceil - \lfloor x \rfloor} = x$$

- The expected value of the computed result is the exact result

$$\begin{aligned} & \mathbb{E}(\mathrm{fl}(a \text{ op } b)) = a \text{ op } b \\ \Rightarrow \quad & \mathbb{E}((a \text{ op } b)(1+\delta)) = a \text{ op } b \\ \Rightarrow \quad & (a \text{ op } b)\,\mathbb{E}(\delta) = 0 \\ \Rightarrow \quad & \mathbb{E}(\delta) = 0 \quad \text{if } a \text{ op } b \neq 0 \end{aligned}$$

$\Rightarrow$ **Stochastic rounding enforces zero mean rounding errors**

Stochastic rounding $\not\Rightarrow$ independent δ_i

- Consider the computation of $s := (a+b)+c$

$$\widehat{s} = \mathrm{fl}(\mathrm{fl}(a+b)+c) = \big((a+b)(1+\delta_1)+c\big)(1+\delta_2)$$

- Define $\widehat{s}_1 = \mathrm{fl}(a+b)+c = (a+b)(1+\delta_1)+c$

- Then, $\delta_2 = \widehat{s} - \widehat{s}_1$ is entirely determined by

$$\delta_2 = \begin{cases} \lceil \widehat{s}_1 \rceil - \widehat{s}_1 \text{ with probability } p = (\widehat{s}_1 - \lfloor \widehat{s}_1 \rfloor)/(\lceil \widehat{s}_1 \rceil - \lfloor \widehat{s}_1 \rfloor), \\ \lfloor \widehat{s}_1 \rfloor - \widehat{s}_1 \text{ with probability } 1-p \end{cases}$$

which clearly depends on $\widehat{s}_1$ and so on δ_1

$\Rightarrow$ **Even with stoch. rounding, rounding errors may be dependent**

Stochastic rounding $\Rightarrow$ mean independent δ_i

- Consider the computation of $s = \widehat{a} \text{ op } \widehat{b}$, where the computation of $\widehat{a}$ and $\widehat{b}$ has already produced k rounding errors $\delta_1, \dots, \delta_k$
- Then, $\widehat{s} = \mathrm{fl}(\widehat{a} \text{ op } \widehat{b}) = (\widehat{a} \text{ op } \widehat{b})(1 + \delta_{k+1})$ and $\delta_{k+1} = \widehat{s} - s$ (which depends on $\delta_1, \dots, \delta_k$) is given by

$$\delta_{k+1} = \begin{cases} \lceil s \rceil - s \text{ with probability } p = \frac{s - \lfloor s \rfloor}{\lceil s \rceil - \lfloor s \rfloor} \\ \lfloor s \rfloor - s \text{ with probability } 1 - p = \frac{\lceil s \rceil - s}{\lceil s \rceil - \lfloor s \rfloor} \end{cases}$$

- Since $\lceil s \rceil - s$ and $\lfloor s \rfloor - s$ are entirely determined by $\delta_1, \dots, \delta_k$

$$\mathbb{E}(\lceil s \rceil - s \mid \delta_1, \dots, \delta_k) = \lceil s \rceil - s$$
$$\mathbb{E}(\lfloor s \rfloor - s \mid \delta_1, \dots, \delta_k) = \lfloor s \rfloor - s$$

  where $\mathbb{E}(X \mid Y)$ denotes the conditional expectation of X given Y
- Therefore we obtain

$$\begin{aligned} \mathbb{E}\left(\delta_{k+1} \mid \delta_1, \dots, \delta_k\right) &= p\, \mathbb{E}\left(\lceil s \rceil - s \mid \delta_1, \dots, \delta_k\right) + (1-p)\, \mathbb{E}\left(\lfloor s \rfloor - s \mid \delta_1, \dots, \delta_k\right) \\ &= p(\lceil s \rceil - s) + (1-p)(\lfloor s \rfloor - s) = 0 \end{aligned}$$

$\Rightarrow$ **Stochastic rounding enforces mean independence:**

$$\mathbb{E}(\delta_i \mid \delta_1, \dots, \delta_{i-1}) = \mathbb{E}(\delta_i) \ (= 0)$$

Martingales and Azuma–Hoeffding inequality

- A sequence of random variables E_0, ..., E_n is called a **martingale** if, for all k, $\mathbb{E}(|E_k|) < \infty$ and $\mathbb{E}(E_{k+1} \mid E_0, \ldots, E_k) = E_k$
- Example: random walks are martingales. Position at step $k+1$ depends on previous positions but, if all directions have equal probabilities, its expected value is the position at step k

Azuma–Hoeffding inequality

Let E_0, ..., E_n be a martingale such that $|E_{k+1} - E_k| \leq c$, for $k = 0\colon n-1$. Then, for any $\lambda > 0$,

$$\Pr\left(|E_n - E_0| \geq \lambda\sqrt{n}c\right) \leq 2\exp(-\lambda^2/2)$$

- Azuma–Hoeffding generalizes Hoeffding's inequality to possibly dependent random variables

$\Rightarrow$ Can we relax our model to mean independent δ_i?

An even more general probabilistic model

Probabilistic model of rounding errors

Let the computation of interest generate rounding errors δ_1, δ_2, ... in that order. The δ_k are (possibly dependent) random variables of mean zero and mean independent of the previous δ_1, ..., δ_{k-1}, i.e., $\mathbb{E}(\delta_k \mid \delta_1, \ldots, \delta_{k-1}) = \mathbb{E}(\delta_k) = 0$.

- **Exercise:** prove that with this model, we recover the probabilistic bound $\prod_{i=1}^{n}(1+\delta_i) = 1+\theta_n, \quad |\theta_n| \le \widetilde{\gamma}_n(\lambda)$

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- $E_n = \sum_{i=1}^{n} \delta_i$ (with $E_0 = 0$) is a martingale

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- **Exercise:** prove that with this model, we recover the probabilistic bound $\prod_{i=1}^{n}(1+\delta_i) = 1+\theta_n, \quad |\theta_n| \le \widetilde{\gamma}_n(\lambda)$
- $E_n = \sum_{i=1}^{n} \delta_i$ (with $E_0 = 0$) is a martingale
  $\Rightarrow$ Clearly $|E_k| \le ku \Rightarrow \mathbb{E}(|E_k|) < \infty$ and

$$\begin{aligned}\mathbb{E}(E_{k+1} \mid E_0, \dots, E_k) &= \mathbb{E}(E_k + \delta_{k+1} \mid \delta_1, \dots, \delta_k) \\ &= \mathbb{E}(E_k \mid \delta_1, \dots, \delta_k) + \mathbb{E}(\delta_{k+1} \mid \delta_1, \dots, \delta_k) = E_k\end{aligned}$$

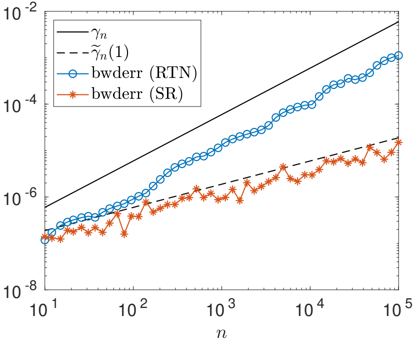
- Azuma–Hoeffding: $|E_{k+1} - E_k| \le u \Rightarrow |E_n - E_0| = |E_n| \le \lambda\sqrt{n}u$
- By Taylor expansions

$$E_n - \frac{nu^2}{1-u} \le \sum_{i=1}^{n} \log(1+\delta_i) \le E_n + \frac{nu^2}{1-u}$$

Stochastic rounding enforces probabilistic bound

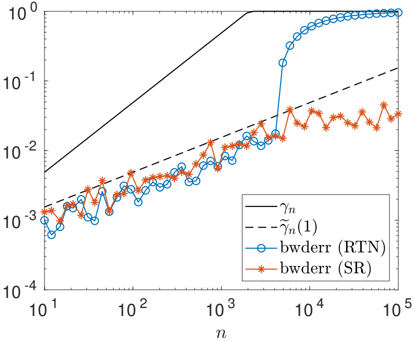
Conclusion: with stochastic rounding,
the probabilistic bound holds rigorously, with no exceptions

Constant x_i (single precision)



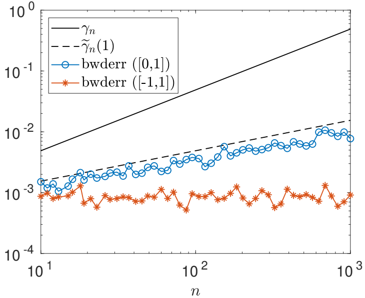
⇒ stochastic rounding produces nonconstant δ_i

Nonzero x_i (half precision)



⇒ stochastic rounding overcomes stagnation

Probabilistic model of the data



We now come back to the observed difference between $[0,1]$ and $[-1,1]$ data

We seek to obtain a **sharper** backward error bound by taking into account the distribution of the x_i

Probabilistic model of the data

The x_i, $i = 1:n$, are independent random variables sampled from a given distribution of mean μ_x and satisfy $|x_i| \le C_x$. In summary, we assume δ_k, x_k, and $x_k\delta_k$ to be mean independent of previous δ_i and x_i:

$$\mathbb{E}(\delta_k \mid \delta_1, \dots, \delta_{k-1}, x_1, \dots, x_{k-1}) = \mathbb{E}(\delta_k) = 0$$

$$\mathbb{E}(x_k \mid \delta_1, \dots, \delta_{k-1}, x_1, \dots, x_{k-1}) = \mathbb{E}(x_k) = \mu_x$$

$$\mathbb{E}(x_k\delta_k \mid \delta_1, \dots, \delta_{k-1}, x_1, \dots, x_{k-1}) = \mathbb{E}(x_k\delta_k) = 0$$

Note that $\mathbb{E}(x_k\delta_k) = 0$ is a consequence of the law of total expectation:

$$\mathbb{E}(x_k\delta_k) = \mathbb{E}(\mathbb{E}(x_k\delta_k|x_k)) = \mathbb{E}(x_k\,\mathbb{E}(\delta_k|x_k))\,\mathbb{E}(x_k\,\mathbb{E}(\delta_k)) = \mathbb{E}(x_k)\,\mathbb{E}(\delta_k) = 0$$

Sharper probabilistic bound for summation

Exercise: compute a bound on the backward error $\frac{|\widehat{s}-s|}{\sum_{i=1}^{n}|x_i|}$

1. Compute an upper bound on $|s_j| = |\sum_{i=1}^{j} x_i|$

2. Compute an upper bound on $|E_n| = |\sum_{j=2}^{n} s_j \delta_j|$

3. Compute a lower bound $\sum_{i=1}^{n} |x_i|$ as a function of $\mu_{|x|}$

Sharper probabilistic bound for summation

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1. Compute an upper bound on $|s_j| = |\sum_{i=1}^{j} x_i|$
   $\Rightarrow$ Hoeffding: $|s_j| \le \mu_x j + \lambda C_x \sqrt{j}$ with prob. $1 - 2\exp(-\lambda^2/2)$
2. Compute an upper bound on $|E_n| = |\sum_{j=2}^{n} s_j \delta_j|$
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2. Compute an upper bound on $|E_n| = |\sum_{j=2}^{n} s_j \delta_j|$
   - Clearly $|E_k| \le k(k-1)C_x u \Rightarrow \mathbb{E}(|E_k|) < \infty$
   - Let $\mathcal{S}_k = \{\delta_1, \ldots, \delta_{k-1}, x_1, \ldots, x_{k-1}\}$, we have

$$\begin{aligned}\mathbb{E}(E_k \mid E_0, \ldots, E_{k-1}) &= \mathbb{E}(E_{k-1} + s_k\delta_k \mid \mathcal{S}_k) \\ &= \mathbb{E}(E_{k-1} \mid \mathcal{S}_k) + \mathbb{E}(s_{k-1}\delta_k \mid \mathcal{S}_k) + \mathbb{E}(x_k\delta_k \mid \mathcal{S}_k) \\ &= E_{k-1} + s_{k-1}\,\mathbb{E}(\delta_k \mid \mathcal{S}_k) + \mathbb{E}(x_k\delta_k \mid \mathcal{S}_k) = E_{k-1}\end{aligned}$$

   - $E_0, \ldots, E_n$ is a martingale and

$$\forall k \le n-1,\ \Pr\Big(|E_{k+1} - E_k| \ge (\mu_x n + \lambda C_x \sqrt{n})u\Big) \le 2\exp(-\lambda^2/2)$$

$$\Rightarrow \Pr\Big(\forall k \le n-1,\ |E_{k+1} - E_k| \ge (\mu_x n + \lambda C_x \sqrt{n})u\Big) \le 2(n-1)\exp(-\lambda^2/2)$$

   $\Rightarrow$ By Azuma–Hoeffding, we obtain with prob. $1 - 2n\exp(-\lambda^2/2)$

$$|\widehat{s} - s| = |E_n - E_0| \le \big(\lambda\mu_x n^{3/2} + \lambda^2 C_x n\big)u$$

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   - $E_0, \dots, E_n$ is a martingale and

$$\forall k \le n{-}1,\ \Pr\Big(|E_{k+1} - E_k| \ge (\mu_x n + \lambda C_x\sqrt{n})u\Big) \le 2\exp(-\lambda^2/2)$$

$$\Rightarrow \Pr\Big(\forall k \le n{-}1,\ |E_{k+1} - E_k| \ge (\mu_x n + \lambda C_x\sqrt{n})u\Big) \le 2(n{-}1)\exp(-\lambda^2/2)$$

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$$|\widehat{s} - s| = |E_n - E_0| \le \big(\lambda\mu_x n^{3/2} + \lambda^2 C_x n\big)u$$

3. Compute a lower bound $\sum_{i=1}^{n}|x_i|$ as a function of $\mu_{|x|}$

   $\Rightarrow$ Hoeffding: $\sum_{i=1}^{n}|x_i| \ge n\mu_{|x|} - \lambda C_x\sqrt{n}$ with prob. $1-2\exp(-\lambda^2/2)$

Sharper probabilistic bound for summation (cont'd)

Main result

Under the previously stated models of rounding errors and data,

$$\varepsilon_{bwd} = \frac{|\widehat{s} - s|}{\sum_{i=1}^n |x_i|} \le \frac{\lambda \mu_x \sqrt{n} + \lambda^2 C_x}{\mu_{|x|} - \lambda C_x/\sqrt{n}} \cdot u + O(u^2)$$

holds with probability $P(\lambda) = 1 - 2(n+1)\exp\left(-\lambda^2/2\right)$

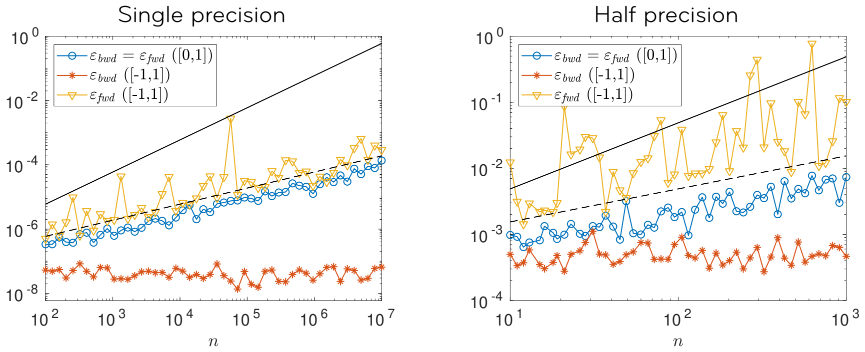
- $\mu_x = O(1) \Rightarrow \varepsilon_{bwd} = O(\sqrt{n}u)$
- $\mu_x = 0$ or $\mu_x \ll 1 \Rightarrow \varepsilon_{bwd} = O(u)$

$$\varepsilon_{fwd} = \kappa \cdot \varepsilon_{bwd}, \qquad \kappa = \frac{\sum_{i=1}^n |x_i|}{\left|\sum_{i=1}^n x_i\right|}$$

What probabilistic bound on κ for random x_i?

- If $\mu_x = \Theta(1)$, $|\sum_{i=1}^n x_i| = \Theta(n)$ and $\sum_{i=1}^n |x_i| = \Theta(n) \Rightarrow \kappa = \Theta(1)$
- If $\mu_x = o(1)$, $|\sum_{i=1}^n x_i| = O(\sqrt{n})$ and $\sum_{i=1}^n |x_i| = \Theta(n) \Rightarrow \kappa = \Omega(\sqrt{n})$

Summary of probabilistic bounds for summation



	General δ_i	Probabilistic model on δ_i (enforced by SR)		
		General x_i	Probabilistic model on x_i	
			$\mu_x \neq 0$	$\mu_x = 0$
κ	—	—	$\Theta(1)$	$\Omega(\sqrt{n})$
ε_{bwd}	nu	$O(\sqrt{n})u$	$\Theta(\sqrt{n})u$	$\Theta(1)u$
ε_{fwd}	$n\kappa u$	$O(\sqrt{n})\kappa u$	$\Theta(\sqrt{n})u$	$\Omega(\sqrt{n})u$

$\sqrt{n}u$ is too large for large n and u! $\Rightarrow$ **we need new algorithms with smaller error bounds** (another story for another time)

Conclusion

Take home message

With the emergence of **large scale computations** and **low precision arithmetics**, **classical analyses can no longer guarantee the numerical stability of classical algorithms**
$\Rightarrow$ **Probabilistic analyses are a powerful and timely tool to obtain sharper error bounds**

Lecture slides available on my webpage

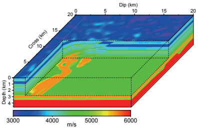
`bit.ly/tmaryLIP6`

To go further

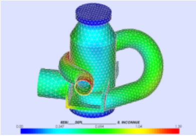
Nicholas J. Higham and Theo Mary, *A New Approach to Probabilistic Rounding Error Analysis*, SIAM Journal on Scientific Computing, 41(5):A2815-A2835, 2019 (PDF available here).

Sujet de stage+thèse: résolution parallèle de problèmes industriels avec techniques de compression multiprécisions (contact: theo.mary@lip6.fr)

- Contexte: les grands défis actuels de la simulation numérique de problèmes industriels de très grande taille requièrent des solveurs linéaires efficaces. Des algorithmes de compression Block Low-Rank (BLR) ont permis de réduire le côut de cette résolution sur architectures parallèles (jusqu'à 2400 coeurs). Exemple de facteurs de compression:



Imagerie sismique
Taille: 130 millions
Précision cible: 10^{-3}
Facteur de compression: 41



Mécanique struct.
Taille: 31 millions
Précision cible: 10^{-9}
Facteur de compression: 26

- Objectif: exploiter les architectures parallèles émergentes conçues pour l'IA (ex: GPU tensor cores) pour décupler ces gains de performance en concevant des algorithmes multiprécisions efficaces qui combinent compression et précisions faibles
- Environnement: le stage (qui pourra se poursuivre en thèse) s'effectuera à Paris (LIP6 et EDF Paris-Saclay) en collaboration avec le groupe MUMPS (Lyon et Toulouse)