Precision-aware Deterministic and Probabilistic Error Bounds for Floating Point Summation

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Abstract We analyze the forward error in the floating point summation of real numbers, for computations in low precision or extreme-scale problem dimensions that push the limits of the precision. We present a systematic recurrence for a martingale on a computational tree, which leads to explicit and interpretable bounds without asymptotic big-O terms. Two probability parameters strengthen the precision-awareness of our bounds: one parameter controls the first order terms in the summation error, while the second one is designed for controlling higher order terms in low precision or extreme-scale problem dimensions. Our systematic approach yields new deterministic and probabilistic error bounds for three classes of mono-precision algorithms: general summation, shifted general summation, and compensated (sequential) summation. Extension of our systematic error analysis to mixed-precision summation algorithms that allow any number of precisions yields the first probabilistic bounds for the mixed-precision FABsum algorithm. Numerical experiments illustrate that the probabilistic bounds are accurate, and that among the three classes of mono-precision algorithms, compensated summation is generally the most accurate. As for mixed precision algorithms, our recommendation is to minimize the magnitude of intermediate partial sums relative to the precision in which they are computed.

Keywords Rounding error analysis \cdot floating-point arithmetic \cdot random variables \cdot martingales \cdot mixed precision \cdot computational tree

Mathematics Subject Classification (2000) 65G99 · 60G42 · 60G50

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1 Introduction

We analyze algorithms for the summation $s_n = x_1 + \cdots + x_n$ in floating point arithmetic of *n* real numbers x_1, \ldots, x_n , and bound the forward error $e_n = \hat{s}_n - s_n$ in the computed sum \hat{s}_n in terms of the unit roundoff *u*.

Our bounds are designed for low precision computations, or extreme-scale problem dimensions n that push the limits of the arithmetic precision with $n > u^{-1}$. The idea is to set up a systematic recurrence for a martingale on a computational tree (Section 2.2), and strengthen its precision-awareness with the help of two probability parameters: one to control the first order terms in the summation error; and a second one to control higher order terms which become more influential with increasing problem dimension or decreasing precision. This precisionaware martingale makes possible a unified and clean derivation of explicit bounds, without asymptotic big-O terms, for a wide variety of mono- and mixed-precison summation algorithms.

As an illustration, we derive new deterministic and probabilistic bounds for three classes of mono-precision algorithms: general summation on a computational tree (Section 2), shifted general summation (Section 3), and compensated summation (Section 4). For compensated summation, our bounds imply that third and higher order terms do not matter, unless the problem dimension n is so extreme as to have already exceeded the limitations of the precision with $n \gg u^{-2}$.

We extend our bounds to mixed-precision summation, allowing any number of precisions, on a computational tree (Section 5). The special case of two precisions leads to the first probabilistic bounds for the mixed-precision FABsum algorithm [2]. Numerical experiments (Section 6) illustrate that the bounds are informative, and that, among the three classes of mono-precision algorithms, compensated summation is the most accurate method.

1.1 Contributions

We present systematic derivations for interpretable precision-aware forward error bounds for summation in mono- and mixed-precision on a computational tree.

Martingales on a computational tree We present a systematic recurrence for martingales on a computational tree (Theorem 2.9, Corollary 2.10), which makes possible a unified and clean derivation of explicit bounds, without asymptotic big-O terms, for a wide variety of summation algorithms.

Our analysis of summation serves as a model problem for systematic error analyses of higher level matrix computations in mixed precision [2], or on hardware with wider accumulators [7].

Precision-aware bounds Our bounds are exact and hold to all orders. This is important when the problem dimension exceeds the precision $n > u^{-1}$; or in low precision, where asymptotic terms $\mathcal{O}(u^2)$ in first-order bounds are too large to be ignored. Precision-awareness is strengthened with two probability parameters: one for controlling the first order terms in the summation error, and a second one for controlling the $\mathcal{O}(u^2)$ terms.

Error bounds for Floating Point Summation

	All Orders	Partial Sums	Martingale	Tree
Higham/Mary [11]	 ✓ 			
Ipsen/Zhou [15]	\checkmark			
Higham/Mary [12]		\checkmark	√	
Connolly/Higham/Mary [4]	\checkmark		\checkmark	
This paper	\checkmark	\checkmark	√	\checkmark

Table 1 A summary of important features in probabilistic error bounds for summation. Check marks in the four columns highlight the presence of the following features: the bounds hold indeed to all orders ('All Orders'); the bounds are expressed in terms of partial sums s_k , thus are tighter than if they had been expressed in terms of inputs x_k ('Partial Sums'); the bounds assume mean-independence of roundoffs rather than the stricter notion of total independence ('Martingale'); the bounds apply to algorithms on any computational tree rather than just sequential summation ('Tree').

General summation on a computational tree We extend the error bounds in [11,15] by customizing them to specific summation algorithms. Rather than depending on the number of inputs n, our bounds depend primarily on the height h of the computational tree, which can be much smaller than n, particularly in parallel computations.

We derive a deterministic bound for the summation error e_n that is proportional to h u (Theorem 2.4) and a probabilistic bound that is proportional to $\sqrt{h} u$. The probabilistic bound treats the roundoffs as zero-mean random variables that are mean-independent (Theorem 2.12, Corollary 2.14) and employs a novel staggered martingale approach in the proof.

Shifted summation algorithms We extend the shifted sequential summation in [2] to shifted general summation (Algorithm 3.1). We derive probabilistic bounds for mean-independent roundoffs (Theorem 3.1).

Compensated summation We derive a recursive expression for the exact error (Theorem 4.1), an explicit expression for the second-order error (Corollary 4.2), and a probabilistic bound (Theorem 4.7) based on our martingale approach. In particular (Remark 4.3) we note the discrepancy by a unit roundoff u of existing bounds with ours,

$$\widehat{s}_n = \sum_{k=1}^n (1+\rho_k) x_k, \qquad |\rho_k| \le 3u + \mathcal{O}(nu^2).$$

Mixed precision summation We present bounds for mixed-precision summation, in any number of precisions, on a computational tree (Theorem 5.2). The special case of two precisions yields the first probabilistic bounds (Corollary 5.3) for the mixed-precision FABsum algorithm [2].

Recommendation For mono- and mixed precision algorithms, pairwise summation based on a balanced binary tree is the most accurate. Furthermore (Remark 5.4), mixed-precision summation should try to minimize the magnitude of the intermediate partial sums s_k relative to the precision u_k in which they are computed, that is, try to minimize $|u_k s_k|$ for all k.

Table 1 summarizes our contributions compared to recent related papers.

1.2 Modeling roundoff

We assume the inputs x_k are floating point numbers, that is, they can be stored exactly without error; and that the summation produces no overflow or underflow. Let 0 < u < 1 denote the unit roundoff to nearest.

Individual roundoffs Apply an operation op $\in \{+, -, *, /\}$ to floating point numbers x and y. In the absence of underflow or overflow, IEEE floating-point arithmetic can be interpreted as computing [10]

$$f(x \text{ op } y) = (x \text{ op } y)(1 + \delta_{xy}), \qquad |\delta_{xy}| \le u.$$
(1.1)

Our probabilistic bounds treat roundoffs as zero-mean mean-independent random variables.

Probabilistic model for sequences of roundoffs Assume the summation generates rounding errors $\delta_1, \delta_2, \ldots$, labeled in a linear order consistent with the partial order of the underlying algorithm. We treat the δ_k as zero-mean random variables that are mean independent¹

$$\mathbb{E}(\delta_k|\delta_1,\dots,\delta_{k-1}) = \mathbb{E}(\delta_k) = 0.$$
(1.2)

Mean-independence (1.2) is a weaker assumption than mutual independence of errors but stronger than uncorrelated errors [12]. At least one mode of stochastic rounding [4] produces the mean-independent errors in (1.2), but the stochastic rounding error bound $|\delta_{xy}| \leq 2u$ is weaker than (1.1).

1.3 Probability theory

For the derivation of the probabilistic bounds, we need a martingale, and a concentration inequality.

Definition 1.1 (Martingale [23]) A sequence of random variables Z_1, \ldots, Z_n is a martingale with respect to the sequence X_1, \ldots, X_n if, for all $k \geq 1$,

- $Z_k \text{ is a function of } X_1, \dots, X_k, \\ \mathbb{E}[|Z_k|] < \infty, \text{ and}$
- $-\mathbb{E}\left[Z_{k+1}|X_1,\ldots,X_k\right] = Z_k.$

Lemma 1.2 (Azuma-Hoeffding inequality [24]) Let Z_1, \ldots, Z_n be a martingale with respect to a sequence X_1, \ldots, X_n , and let c_k be constants with

$$|Z_k - Z_{k-1}| \le c_k, \qquad 2 \le k \le n.$$

Then for any $0 < \delta < 1$, with probability at least $1 - \delta$,

$$|Z_n - Z_1| \le \left(\sum_{k=2}^n c_k^2\right)^{1/2} \sqrt{2\ln(2/\delta)}.$$
(1.3)

¹ For simplicity, the conditioning also includes also those δ_{ℓ} , $1 \leq \ell \leq k - 1$, that are not descendants in the partial order. With stochastic rounding such δ_{ℓ} would be fully independent from δ_k .

If one or more of bounds $|Z_k - Z_{k-1}| \le c_k$ are permitted to fail with probability at most η , then a similar but weaker version of the Azuma-Hoeffding inequality still holds.

Lemma 1.3 (Relaxed Azuma-Hoeffding inequality [3]) Let $0 < \eta < 1$; $0 < \delta < \beta$ 1; and Z_1, \ldots, Z_n be a martingale with respect to a sequence X_1, \ldots, X_n . Let c_k be constants so that all bounds

$$|Z_k - Z_{k-1}| \le c_k, \qquad 2 \le k \le n.$$

hold simultaneously with probability at least $1 - \eta$. Then with probability at least $1 - \eta$ $(\delta + \eta),$

$$|Z_n - Z_1| \le \left(\sum_{k=2}^n c_k^2\right)^{1/2} \sqrt{2\ln(2/\delta)}.$$
(1.4)

2 General summation on a computational tree

We present the algorithm for general summation (Algorithm 2.1); define its computational tree (Definition 2.1); and derive error expressions and a deterministic error bound (Section 2.1); and finally set up a martingale on a computational tree (Section 2.2).

Algorithm 2.1 General summation [10, Algorithm 4.1]

- **Input:** A set of floating point numbers $S = \{x_1, \dots, x_n\}$ **Output:** $s_n = \sum_{k=1}^n x_k$ 1: for k = 2 : n do 2: Remove two elements x and y from S3: $s_k = x + y$ Add s_k to \mathcal{S}
- 4:5: end for

Denote by $s_k = \sum_{j=1}^k x_j$ the exact partial sum, by \hat{s}_k the sum computed in floating point arithmetic, and by $e_k = \hat{s}_k - s_k$ the absolute forward error, $2 \le k \le n$.

Definition 2.1 (Computational tree for Algorithm 2.1) The partial order of pairwise summations in Algorithm 2.1 is represented by a binary tree with 2n - 1 vertices: n-1 pairwise sums s_2, \ldots, s_n to sum n inputs x_1, \ldots, x_n . Specifically,

- Each vertex represents a pairwise sum s_k or an input x_k .
- The root is the final sum s_n , and the leaves are the inputs x_1, \ldots, x_n .
- Each pairwise sum $s_k = x + y$ is a vertex with downward edges (s_k, x) and (s_k, y) . Vertices x and y are the children of s_k .

The tree defines a partial ordering. We say $j \prec k$ if s_j is a descendant of s_k , and $j \preceq k$ if $s_j = s_k$ is possible.

- The height of a node is the length of the longest downward path from that node to a leaf.
- Leaves have height zero.



Fig. 1 Computational trees for two different summation orderings in Algorithm 2.1 for n = 4. Left: sequential (a.k.a. recursive) summation. Right: pairwise summation.

- The height of the tree is the height of its root. Sequential summation yields a tree of height n - 1.

Algorithm 2.1 imposes a *topological ordering* on the graph: $j \prec k$ implies that j < k. Thus if the nodes are visited in the order s_2, \ldots, s_n , no node is visited before its children. Figure 1 shows two computational trees, one of height n-1 for sequential summation; and another of height $\lceil \log_2 n \rceil$ for pairwise summation.

To make our bounds as tight as possible, we express them in terms of partial sums. However, the dependence on the height of the computational tree is more explicit when the bounds are expressed in terms of the inputs. Below is the translation from partial sums to inputs.

Lemma 2.2 (Relation between partial sums and inputs) If h is the height of the computational tree in Algorithm 2.1, then

$$\sum_{k=2}^{n} |s_k| \le h \sum_{j=1}^{n} |x_j|, \qquad \sqrt{\sum_{k=2}^{n} s_k^2} \le \sqrt{h} \sum_{j=1}^{n} |x_j|.$$

Proof The first bound follows from the triangle inequality:

$$\sum_{k=2}^{n} |s_k| \le \sum_{k=2}^{n} \sum_{j \prec k} |x_j| \le \sum_{j=1}^{n} \sum_{j \prec k \preceq n} |x_j| \le h \sum_{j=1}^{n} |x_j|,$$

where in this context $j \prec k$ denotes the set of all leaves x_j that are descendants of node k. The second bound follows from the first:

$$\sum_{k=2}^{n} s_k^2 \le \max_{2 \le j \le n} |s_j| \sum_{k=2}^{n} |s_k| \le \left(\sum_{j=1}^{n} |x_j|\right) \left(h \sum_{j=1}^{n} |x_j|\right) = h\left(\sum_{j=1}^{n} |x_j|\right)^2.$$

2.1 Explicit expressions and deterministic bounds for errors on computational trees

We present two expressions for the error in Algorithm 2.1 (Lemmas 2.3 and 2.6), and a deterministic bound (Theorem 2.4).

We generalize the error for sequential summation in [9, Lemma 3.1] to errors on computational trees. Lemma 2.3 (First explicit expression) The error in Algorithm 2.1 equals

$$e_n = \hat{s}_n - s_n = \sum_{k=2}^n s_k \delta_k \prod_{k \prec j \preceq n} (1 + \delta_j).$$
(2.1)

Lemma 2.3 represents the forward error as a sum of local errors at a node, each perturbed by subsequent rounding errors. Truncating (2.1) yields the first order bound

$$e_n = \sum_{k=2}^n s_k \delta_k + \mathcal{O}(u^2), \qquad (2.2)$$

which extends the result for sequential summation [12, Lemma 2.1]. Lemma 2.3 also allows us to conveniently obtain a deterministic error bound.

Theorem 2.4 If h is the height of the computational tree for Algorithm 2.1 and $\lambda_h \equiv (1+u)^h$, then the error in Algorithm 2.1 is bounded by

$$|e_n| \le \sum_{k=2}^n |s_k| |\delta_k| \prod_{k \prec j \preceq n} |1 + \delta_j| \le \lambda_h u \sum_{k=2}^n |s_k|$$
$$\le \lambda_h h u \sum_{j=1}^n |x_j|.$$

Proof The first bound is a direct consequence of Lemma 2.3, while the last bound follows from Lemma 2.2.

Remark 2.5 A bound [10, (4.3)] similar to the first one in Theorem 2.4,

$$|e_n| \le u \sum_{k=2}^n |\widehat{s}_k|,$$

is accompanied by the following observation:

In designing or choosing a summation method to achieve high accuracy, the aim should be to minimize the absolute values of the intermediate sums s_k .

Reducing the height of the computational tree often helps in this regard. The dependence on the height h is explicitly visible in the second bound of Theorem 2.4.

Since the sum in Lemma 2.3 is not a martingale with respect to the errors $\delta_2, \ldots, \delta_n$, we present an alternative geared towards the error model (1.2): The sum in Lemma 2.6 is a martingale if summed in the original order, as shown in Section 2.2. Lemma 2.6 also expresses the error in terms of exact partial sums, thereby making it more amenable to a probabilistic analysis than the computed partial sums in $e_n = \sum_{k=2}^n \hat{s}_k \tilde{\delta}_k$ [10, (4.2)].

Lemma 2.6 (Second explicit expression) The error in Algorithm 2.1 equals

$$e_n = \hat{s}_n - s_n = \sum_{j=2}^n (s_j + f_j)\delta_j,$$
 (2.3)

where $f_j = 0$ for all nodes whose children are leaves, that is, represent a sum of two inputs x_i and x_j . For all other nodes, the child-errors satisfy the recurrence

$$f_k \equiv \sum_{j \prec k} (s_j + f_j) \delta_j. \tag{2.4}$$

Proof Express the computed parent sum in line 3 of Algorithm 2.1 as the sum of the computed children $\hat{x} = x + e_x$ and $\hat{y} = y + e_y$,

$$\widehat{s}_k = (\widehat{x} + \widehat{y})(1 + \delta_k), \qquad 2 \le k \le n,$$

where $e_x = e_y = 0$ if x and y are inputs x_i and x_j . Highlight the error in the computed children,

$$s_k + e_k = \hat{s}_k = ((x + e_x) + (y + e_y))(1 + \delta_k) = (s_k + e_x + e_y)(1 + \delta_k)$$

= $\underbrace{(e_x + e_y)}_{f_k}(1 + \delta_k) + s_k\delta_k + s_k$

to obtain the error in the computed parent

$$e_k = f_k + (s_k + f_k)\delta_k, \qquad 2 \le k \le n.$$

Now unravel the recurrence for f_k , where $f_j = 0$ for all nodes j with two leaf children.

We refer to the terms f_k as *child-errors*, since at any given node, f_k is equal to the sum of the errors in the computed children.

Example 2.7 A pairwise tree summation for n = 8 illustrates the recurrences for the child-errors in Lemma 2.6.

1. Sums of leaf nodes: The exact sums are

$$s_2 = x_1 + x_2$$
, $s_3 = x_3 + x_4$, $s_4 = x_5 + x_6$, $s_5 = x_7 + x_8$,

while the computed sums are $\hat{s}_j = s_j + s_j \delta_j$ with child-errors $f_j = 0$ for $2 \le j \le 5$. 2. Second level: The exact sums are $s_6 = s_2 + s_3$ and $s_7 = s_4 + s_5$ while the computed

2. Second level: The exact sums are $s_6 = s_2 + s_3$ and $s_7 = s_4 + s_5$ while the computed sums are

$$\hat{s}_{6} = (\hat{s}_{2} + \hat{s}_{3})(1 + \delta_{6}) = \underbrace{(s_{2}\delta_{2} + s_{3}\delta_{3})}_{f_{6}}(1 + \delta_{6}) + s_{6}\delta_{6} + s_{6}$$

$$= f_{6} + (s_{6} + f_{6})\delta_{6} + s_{6}$$

$$\hat{s}_{7} = (\hat{s}_{4} + \hat{s}_{5})(1 + \delta_{7}) = \underbrace{(s_{4}\delta_{4} + s_{5}\delta_{5})}_{f_{7}}(1 + \delta_{7}) + s_{7}\delta_{7} + s_{7}$$

$$= f_{7} + (s_{7} + f_{7})\delta_{7} + s_{7}.$$

With $f_j = 0, \ 2 \le j \le 5$, the child-errors are

$$f_6 = s_2 \delta_2 + s_3 \delta_3 = (s_2 + f_2) \delta_2 + (s_3 + f_3) \delta_3 = \sum_{j \prec 6} (s_j + f_j) \delta_j$$

$$f_7 = s_4 \delta_4 + s_5 \delta_5 = (s_4 + f_4) \delta_4 + (s_5 + f_5) \delta_5 = \sum_{j \prec 7} (s_j + f_j) \delta_j$$

3. Final level: The exact sum is $s_8 = s_6 + s_7$ while the computed sum is

$$\hat{s}_8 = (\hat{s}_6 + \hat{s}_7)(1 + \delta_8)$$

= $\underbrace{(f_6 + (s_6 + f_6)\delta_6 + f_7 + (s_7 + f_7)\delta_7)}_{f_8}(1 + \delta_8) + s_8\delta_8 + s_8$
= $f_8 + (s_8 + f_8)\delta_8 + s_8,$

with child-error

$$f_8 = f_6 + f_7 + (s_6 + f_6)\delta_6 + (s_7 + f_7)\delta_7$$

= $\sum_{j=2}^5 (s_j + f_j)\delta_j + (s_6 + f_6)\delta_6 + (s_7 + f_7)\delta_7 = \sum_{j=2}^7 (s_j + f_j)\delta_j.$

The total error is

$$e_8 = f_8 + (s_8 + f_8)\delta_8 = \sum_{j=2}^7 (s_j + f_j)\delta_j + (s_8 + f_8)\delta_8 = \sum_{j=2}^8 (s_j + f_j)\delta_j.$$

2.2 Setting up martingales on computational trees

We derive a probabilistic bound (Lemma 2.8) for the child-errors in Lemma 2.6, followed by two types of probabilistic bounds for the error in Algorithm 2.1: one in terms of a recurrence relation (Theorem 2.9 and Corollary 2.10) and a second in closed form (Theorem 2.12 and Corollary 2.14).

We introduce our first probability parameter η which controls terms of order two and higher in e_n , and guarantees, with probability at least $1 - \eta$, that all child errors $|f_k|$ are simultaneously bounded.

Lemma 2.8 Let L be the number of nodes in the computational tree whose children are both leaves, and let $\tilde{n} \equiv n - L - 1$ be the number of nodes with at least one non-leaf child. Without loss of generality let nodes $2, \ldots, L+1$ be the ones with two leaf children. Let $0 < \eta < 1$ and $\lambda_{\tilde{n},\eta} \equiv \sqrt{2 \ln(2\tilde{n}/\eta)}$. Then under (1.2), with probability at least $1 - \eta$, the child errors in (2.4) are bounded by

$$|f_k| \le F_{k,\tilde{n},\eta}, \qquad 2 \le k \le n$$

where

$$F_{k,\tilde{n},\eta} = \begin{cases} 0 & 2 \le k \le L+1, \\ \lambda_{\tilde{n},\eta} u \left(\sum_{j \prec k} (|s_j| + F_{j,\tilde{n},\eta})^2 \right)^{1/2} & L+2 \le k \le n, \end{cases}$$
(2.5)

Proof This is an induction proof over k and the failure probability η .

Induction basis $2 \le k \le L+1$ Since the inputs (leaves) are assumed to be exact, $f_k \equiv 0$ in (2.4). Thus $|f_k| \le F_{k,\tilde{n},\eta}$ clearly holds.

Induction hypothesis Assume that the k-2 bounds

$$|f_j| \le F_{j,\tilde{n},\eta}, \qquad 2 \le j \le k-1$$

hold simultaneously with probability at least $1 - \frac{k-L-2}{\tilde{n}}\eta$.

Induction step Move the precedence relation $j \prec k$ inside the sum, in order to write the child-error recurrence (2.4) as a contiguous sum,

$$f_k = \sum_{j=2}^{k-1} (s_j + f_j) \delta_j \mathbb{1}_{j \prec k}.$$

With $\delta_1 = 0$, the sequence $Z_1 \equiv 0$, $Z_i \equiv \sum_{j=2}^{i} (s_j + f_j) \delta_j \mathbb{1}_{j \prec k}$, $2 \leq i \leq k-1$, is a martingale with respect to $\delta_1, \ldots, \delta_{k-1}$. According to the induction hypothesis, the k-2 bounds

$$|Z_i - Z_{i-1}| \le \begin{cases} u(|s_i| + F_{i,\tilde{n},\eta}) & i \prec k, \\ 0 & i \not\prec k, \end{cases} \qquad 2 \le i \le k-1,$$

hold simultaneously with probability at least $1 - \frac{k-L-2}{\tilde{n}}\eta$. Since $f_k = Z_{k-1} - Z_1$, setting $\delta = \eta/\tilde{n}$, Lemma 1.2 implies that with probability at least $1 - \delta$

$$|f_k| \le \lambda_{\tilde{n},\eta} u \left(\sum_{j \prec k} (|s_j| + F_{j,\tilde{n},\eta})^2 \right)^{1/2} = F_{k,\tilde{n},\eta}.$$

So $|f_j| \leq F_{j,\tilde{n},\eta}$ hold simultaneously for $2 \leq j \leq k$ with probability at least $1 - \frac{k-L-1}{\tilde{n}}\eta$. By induction, $|f_k| \leq F_{k,\tilde{n},\eta}$ holds for $2 \leq k \leq n$ with probability at least $1 - \eta$.

Sequential summation has L = 1 nodes both of whose children are leaves, while pairwise summation has $L = \lfloor n/2 \rfloor$.

Finally we are ready for setting up a martingale on a computational tree, where a second probability parameter δ controls the first-order terms in e_n .

Theorem 2.9 Let $0 < \eta < 1$; $0 < \delta < 1 - \eta$; and $F_{j,\tilde{n},\eta}$ defined as in (2.5). Then under the model (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 2.1 is bounded by

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(\sum_{j=2}^n (|s_j| + F_{j,\tilde{n},\eta})^2\right)^{1/2}.$$
 (2.6)

Proof Write the error as in (2.3),

$$e_n = \sum_{j=2}^n (s_j + f_j) \delta_j.$$

With $\delta_1 = 0$, the sequence $Z_1 \equiv 0$, $Z_i \equiv \sum_{j=2}^i (s_j + f_j) \delta_j$, $2 \le i \le n$, is a martingale with respect to $\delta_1, \ldots, \delta_n$. Lemma 2.8 implies that with probability at least $1 - \eta$, the bounds $|f_j| \le F_{j,\tilde{n},\eta}$ hold simultaneously for $2 \le j \le n$. Thus with probability at least $1 - \eta$, the martingale differences are bounded by

$$|Z_i - Z_{i-1}| = |(s_i + f_i)\delta_i| \le u(|s_i| + F_{i,\tilde{n},\eta}), \qquad 2 \le i \le n.$$

At last, Lemma 1.3 implies that (2.6) holds with probability at least $1 - (\delta + \eta)$.

Below is a simpler bound that holds for every summation algorithm and does not require knowledge of the number L of nodes with two leaf children. Its first-order version illustrates the absence of η from the first-order error term.

Corollary 2.10 Let $0 < \eta < 1$ and $0 < \delta < 1 - \eta$. Then under (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 2.1 is bounded by

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(\sum_{j=2}^n (|s_j| + F_{j,n,\eta})^2\right)^{1/2}$$

= $u\sqrt{2\ln(2/\delta)} \sqrt{\sum_{k=2}^n s_k^2} + \mathcal{O}(u^2),$

where $F_{2,n,\eta} \equiv 0$ and $F_{k,n,\eta} \equiv \lambda_{n,\eta} u \left(\sum_{j \prec k} (|s_j| + F_{j,n,\eta})^2 \right)^{1/2}, \ 3 \le k \le n.$

Remark 2.11 We present the following novel approach for proving Theorem 2.12.

- 1. Write the forward errors e_k in terms of child-errors f_k (see Lemma 2.6).
- 2. Express each f_k as a martingale in terms of the preceding child-errors, and repeatedly use the Azuma-Hoeffding inequality in Lemma 1.2 to bound all of them simultaneously with probability at least 1η (see Lemma 2.8).
- 3. Express the error e_n as a martingale whose bounds depend on the f_k bounds, and then derive a bound for $|e_n|$ that holds with probability at least $1 - (\eta + \delta)$ (see Theorem 2.9).
- 4. Simplify the bound through repeated applications of the triangle inequality.

Theorem 2.12 Let $0 < \eta < 1$; $0 < \delta < 1 - \eta$, and \tilde{n} the number of nodes with two non-leaf children. Then under the model (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 2.1 is bounded by

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(1 + \phi_{\tilde{n},h,\eta}\right) \sqrt{\sum_{k=2}^n s_k^2}$$
$$\le u\sqrt{h}\sqrt{2\ln(2/\delta)} \left(1 + \phi_{\tilde{n},h,\eta}\right) \sum_{k=1}^n |x_k|,$$

where h is the height of the computational tree and

$$\phi_{\tilde{n},h,\eta} \equiv \lambda_{\tilde{n},\eta} \sqrt{2h} \, u \, \exp\left(\lambda_{\tilde{n},\eta}^2 h u^2\right) \qquad \text{with} \qquad \lambda_{\tilde{n},\eta} \equiv \sqrt{2\ln(2\tilde{n}/\eta)}. \tag{2.7}$$

Proof Apply the 2-norm triangle inequality to the sum in Theorem 2.9,

$$\left(\sum_{j_1=2}^n (|s_{j_1}| + F_{j_1,\tilde{n},\eta})^2\right)^{1/2} \le \sqrt{\sum_{k=2}^n s_k^2} + \left(\sum_{j_1 \le n} F_{j_1,\tilde{n},\eta}^2\right)^{1/2}$$

Apply the recurrence for $F_{j,\tilde{n},\eta}$ from (2.5), followed by the triangle inequality,

$$\left(\sum_{j_{1} \leq n} F_{j_{1},\tilde{n},\eta}^{2}\right)^{1/2} = \left(\sum_{j_{1} \leq n} \sum_{j_{2} \prec j_{1}} \lambda_{\tilde{n},\eta}^{2} u^{2} (|s_{j_{2}}| + F_{j_{2},\tilde{n},\eta})^{2}\right)^{1/2}$$

$$\leq \lambda_{\tilde{n},\eta} u \sqrt{\sum_{j_{2} \prec j_{1} \leq n} s_{j_{2}}^{2}} + \lambda_{\tilde{n},\eta} u \left(\sum_{j_{2} \prec j_{1} \leq n} F_{j_{2},\tilde{n},\eta}^{2}\right)^{1/2}$$

$$\leq \lambda_{\tilde{n},\eta} u \sqrt{\binom{h}{1}} \sqrt{\sum_{k=2}^{n} s_{k}^{2}} + \lambda_{\tilde{n},\eta} u \left(\sum_{j_{2} \prec j_{1} \leq n} F_{j_{2},\tilde{n},\eta}^{2}\right)^{1/2},$$

where the final inequality follows from the fact that for each index j_2 , there are at most h possibilities for the index j_1 , thus each partial sum s_k appears at most h times. Repeating this and combining the result with Theorem 2.9 shows that with probability at least $1 - (\delta + \eta)$ the error is bounded by

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(\sum_{j=0}^h \lambda_{\tilde{n},\eta}^j u^j \sqrt{\binom{h}{j}}\right) \sqrt{\sum_{k=2}^n s_k^2}.$$
 (2.8)

Next, we bound the sum by a simpler expression. Set $\gamma_j \equiv 2^j$ for $1 \leq j \leq h$. The Cauchy-Schwarz inequality implies that

$$\left(\sum_{j=1}^{h} x_j\right)^2 = \left(\sum_{j=1}^{h} \frac{1}{\sqrt{\gamma_j}} \cdot \sqrt{\gamma_j} x_j\right)^2 \le \left(\sum_{j=1}^{h} \frac{1}{\gamma_j}\right) \left(\sum_{j=1}^{h} \gamma_j x_j^2\right) \le \sum_{j=1}^{h} \gamma_j x_j^2.$$
(2.9)

Thus,

$$\sum_{j=1}^{h} \lambda_{\bar{n},\eta}^{j} u^{j} \sqrt{\binom{h}{j}} \leq \left(\sum_{j=1}^{h} 2^{j} \lambda_{\bar{n},\eta}^{2j} u^{2j} \binom{h}{j}\right)^{1/2} = \sqrt{(1+2\lambda_{\bar{n},\eta}^{2} u^{2})^{h} - 1}$$
$$\leq \sqrt{\exp\left(2\lambda_{\bar{n},\eta}^{2} h u^{2}\right) - 1}$$
$$\leq \sqrt{2\lambda_{\bar{n},\eta}^{2} h u^{2} \exp\left(2\lambda_{\bar{n},\eta}^{2} h u^{2}\right)} = \phi_{\bar{n},h,\eta}.$$

Substituting this bound into (2.8) gives the desired result.

Theorem 2.12 implies that with high probability the summation error to first order is proportional to \sqrt{h} , where h is the height of the computational tree. This confirms that even under the probabilistic model, summation algorithms based on shallow computational trees are likely to be more accurate.

Remark 2.13 The quantity $\phi_{\bar{n},h,\eta}$ appears only in second and higher order terms of the error, and might possibly become significant only if the computational tree is deep enough so that $\lambda_{\bar{n},\eta}\sqrt{2hu} \approx 1$. However, the effect of η on the overall bound, even under adverse circumstances, is negligible.

Consider single precision computation where $u = 2^{-24} \approx 5.96 \cdot 10^{-8}$. Assume an extreme problem size $n = 10^{10}$ with a computational tree of maximal height h = n, and a tremendously strict probability $\eta = 10^{-32}$. Then $\lambda_{\bar{n},\eta} \approx 14.0$, and $\exp(\lambda_{\bar{n},\eta}^2 hu^2) = 1$ to three digits, so that the total contribution of the higher order terms is merely a factor of $1 + \phi_{\bar{n},h,\eta} < 1.12$.

In the special case of sequential summation, the first bound in Theorem 2.12 is stronger than [12, Theorem 2.4], while the second bound shows agreement to first order.

For completeness, we present a simpler bound that holds for all summation algorithms and does not require knowledge of the number of nodes L with two leaf children.

Corollary 2.14 Let $0 < \eta < 1$; $0 < \delta < 1 - \eta$. Then under the model (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 2.1 is bounded by

$$\begin{aligned} |e_n| &\leq u\sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,h,\eta}\right) \sqrt{\sum_{k=2}^n s_k^2} \\ &\leq u\sqrt{h}\sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,h,\eta}\right) \sum_{k=1}^n |x_k|, \end{aligned}$$

where h is the height of the computational tree and

$$\phi_{n,h,\eta} \equiv \lambda_{n,\eta} \sqrt{2h} \, u \, \exp\left(\lambda_{n,\eta}^2 h u^2\right) \qquad \text{with} \qquad \lambda_{n,\eta} \equiv \sqrt{2\ln(2n/\eta)}. \tag{2.10}$$

3 Shifted summation

We present an algorithm for shifted summation (Algorithm 3.1) which centers the inputs x_j , and derive a probabilistic error bound (Theorem 3.1).

Shifted summation is motivated by work in computer architecture [5,6] and formal methods for program verification [22] where not only the roundoffs but also the inputs are interpreted as random variables sampled from some distribution. Then one can compute statistics for the total roundoff error and estimate the probability that it is bounded by tu for a given t.

Probabilistic bounds for random inputs are derived in [12], with improvements in [9], to show that sequential summation is accurate for inputs x_j that are tightly clustered around zero. As a consequence, accuracy can be improved by shifting the inputs to have zero mean, which is affordable in the context of matrix multiplication [12, Section 4].

Our Algorithm 3.1 extends the shifted algorithm for sequential summation [12, Algorithm 4.1] to general summation. Figure 2 shows the computational tree for n = 2.

The pseudo-code in Algorithm 3.1 is geared towards exposition. In practice, one shifts the x_k immediately prior to the summation, to avoid allocating additional storage for $y_k = x_k - c$. The ideal choice for centering is the empirical mean $c = s_n/n$. A simpler approximation is $c = (\min_k x_k + \max_k x_k)/2$.

Error bounds for Algorithm 3.1 follow almost directly from the ones for Algorithm 2.1. Figure 2 shows the associated computational tree for n = 2. It has

Algorithm 3.1 Shifted General Summation

Input: Floating point numbers x_1, \ldots, x_n ; shift c **Output:** $s_n = \sum_{k=1}^n x_k$ 1: for k = 1 : n do 2: $y_k = x_k - c$ 3: end for 4: $y_{n+1} = nc$ 5: t_n = output of Algorithm 2.1 applied to y_1, \ldots, y_n

6: return $s_n = t_n + y_{n+1}$



Fig. 2 Computational tree for shifted summation, n = 2. The dotted boundary delineates the inputs of and summations computed by the call to Algorithm 2.1 in line 5 of Algorithm 3.1.

4n+3 vertices, and its height is equal to two plus the height of the tree in the call to Algorithm 2.1. The one twist is the additional multiplication y = nc, but if n and c can be stored exactly then the error analysis remains the same.²

Theorem 3.1 Let $0 < \eta < 1$; $0 < \delta < 1 - \eta$. Then under the model (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 3.1 is bounded by

$$|e_{n}| \leq u\sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,h,\eta}\right) \sqrt{s_{n}^{2} + \sum_{k=2}^{n} t_{k}^{2} + \sum_{k=1}^{n+1} y_{k}^{2}}$$
$$\leq u\sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,h,\eta}\right) \left(n|c| + \sqrt{h} \sum_{k=1}^{n} \left(|x_{k} - c| + |x_{k}|\right)\right)$$

where h is the height of the computational tree and $\phi_{n,h,\eta}$ is defined in (2.10).

With regard to the factor $\lambda_{n,\eta} \equiv \sqrt{2\ln(2n/\eta)}$ in $\phi_{n,h,\eta}$, the tree for Algorithm 3.1 has L = n nodes both of whose children are leaves.

4 Compensated sequential summation

Our approach is not restricted to algorithms whose computational graphs are trees, and we demonstrate its versatility by analyzing the forward error for compensated sequential summation (Algorithm 4.1). After deriving exact error expressions (Section 4.1) and bounds that hold to second order (Section 4.2), we derive an exact probabilistic bound (Section 4.3).

Algorithm 4.1 is the formulation [8, Theorem 8] of the 'Kahan Summation Formula' [18]. A version with opposite signs is presented in [10, Algorithm 4.2].

 $^{^2}$ If n does not admit an exact floating point representation, then we could append an additional node for the artificial 'addition' n + 0, which simulates the rounding of n.

Algorithm 4.1 Compensated Summation [8, Theorem 8] [19, page 9-4] Input: Floating point numbers x_1, \ldots, x_n Output: $s_n = \sum_{k=1}^n x_k$ 1: $s_1 = x_1, c_1 = 0$ 2: for k = 2: n do 3: $y_k = x_k - c_{k-1}$ 4: $s_k = s_{k-1} + y_k$ 5: $c_k = (s_k - s_{k-1}) - y_k$ 6: end for 7: return s_n

Following [19, page 9-5] and additionally defining the computed terms $\widehat{z}_k,$ our finite precision model of Algorithm 4.1 is

$$\hat{s}_{1} = s_{1} = x_{1}, \quad \hat{c}_{1} = 0, \quad \eta_{2} = 0
\hat{y}_{k} = (x_{k} - \hat{c}_{k-1})(1 + \eta_{k}), \quad 2 \le k \le n
\hat{s}_{k} = (\hat{s}_{k-1} + \hat{y}_{k})(1 + \sigma_{k})
\hat{z}_{k} = (\hat{s}_{k} - \hat{s}_{k-1})(1 + \delta_{k})
\hat{c}_{k} = (\hat{z}_{k} - \hat{y}_{k})(1 + \beta_{k}),$$
(4.1)

4.1 Error expressions

Mimicking the strategy for general summation, we derive an analogue of Lemma 2.6 for compensated summation. We use single dots to represent individual forward errors³,

$$\dot{y}_k \equiv \hat{y}_k - x_k, \qquad \dot{s}_k \equiv \hat{s}_k - s_k, \qquad \dot{z}_k \equiv \hat{z}_k - x_k, \qquad \dot{c}_k \equiv \hat{c}_k, \qquad (4.2)$$

and double dots to represent child-errors,

$$\ddot{y}_k \equiv -\dot{c}_{k-1}, \qquad \ddot{s}_k \equiv \dot{s}_{k-1} + \dot{y}_k, \qquad \ddot{z}_k \equiv \dot{s}_k - \dot{s}_{k-1}, \qquad \ddot{c}_k \equiv \dot{z}_k - \dot{y}_k.$$
 (4.3)

The relations (4.1) imply the forward error recursions

$$\dot{y}_k = (x_k + \ddot{y}_k)\eta_k + \ddot{y}_k,\tag{4.4a}$$

$$\dot{s}_k = (s_k + \ddot{s}_k)\sigma_k + \ddot{s}_k,\tag{4.4b}$$

$$\dot{z}_k = (x_k + \ddot{z}_k)\delta_k + \ddot{z}_k, \qquad (4.4c)$$

$$\dot{c}_k = \ddot{c}_k \beta_k + \ddot{c}_k. \tag{4.4d}$$

Now we derive recurrence relations for the child-errors. Fortunately, the recurrences for \ddot{y}_k , \ddot{z}_k , and \ddot{c}_k are mercifully short, with a length independent of k.

Theorem 4.1 The child-errors in Algorithm 4.1 equal

$$\ddot{y}_2 = 0, \qquad \ddot{s}_2 = 0, \qquad \ddot{z}_2 = s_2 \sigma_2, \qquad \ddot{c}_2 = (x_2 + \ddot{z}_2)\delta_2 + s_2 \sigma_2, \qquad (4.5)$$

 $^{^{3}\,}$ The dots do not refer to differentiation!

and for $3 \leq k \leq n$,

$$\ddot{y}_k = -\ddot{c}_{k-1}(1+\beta_{k-1}), \tag{4.6a}$$

$$\ddot{s}_k = \sum_{j=3}^{n} (x_j + \ddot{y}_j)\eta_j - \ddot{c}_{j-1}\beta_{j-1} - (x_{j-1} + \ddot{z}_{j-1})\delta_{j-1}, \qquad (4.6b)$$

$$\ddot{z}_k = (s_k + \ddot{s}_k)\sigma_k + (x_k + \ddot{y}_k)\eta_k + \ddot{y}_k, \qquad (4.6c)$$

$$\ddot{c}_k = (x_k + \ddot{z}_k)\delta_k + (s_k + \ddot{s}_k)\sigma_k.$$
(4.6d)

Proof First, (4.6a) follows directly from (4.3) and (4.4d). Second,

$$\begin{aligned} \ddot{c}_{k} &= \dot{z}_{k} - \dot{y}_{k} & \text{by (4.3)} \\ &= (x_{k} + \ddot{z}_{k})\delta_{k} + \ddot{z}_{k} - \dot{y}_{k} & \text{by (4.4c)} \\ &= (x_{k} + \ddot{z}_{k})\delta_{k} + \dot{s}_{k} - \dot{s}_{k-1} - \dot{y}_{k} & \text{by (4.3)} \\ &= (x_{k} + \ddot{z}_{k})\delta_{k} + (s_{k} + \ddot{s}_{k})\sigma_{k} + \ddot{s}_{k} - (\dot{s}_{k-1} + \dot{y}_{k}) & \text{by (4.4b)} \\ &= (x_{k} + \ddot{z}_{k})\delta_{k} + (s_{k} + \ddot{s}_{k})\sigma_{k}, & \text{by (4.3)} \end{aligned}$$

which establishes (4.6d). Third,

$$\begin{split} \ddot{s}_{k} &= \dot{s}_{k-1} + \dot{y}_{k} & \text{by (4.3)} \\ &= \ddot{s}_{k-1} + (s_{k-1} + \ddot{s}_{k-1})\sigma_{k-1} + (x_{k} + \ddot{y}_{k})\eta_{k} + \ddot{y}_{k} & \text{by (4.4a), (4.4b)} \\ &= \ddot{s}_{k-1} + (s_{k-1} + \ddot{s}_{k-1})\sigma_{k-1} + (x_{k} + \ddot{y}_{k})\eta_{k} - \ddot{c}_{k-1}(1 + \beta_{k-1}) & \text{by (4.6a)} \\ &= \ddot{s}_{k-1} + (x_{k} + \ddot{y}_{k})\eta_{k} - \ddot{c}_{k-1}\beta_{k-1} - (x_{k-1} + \ddot{z}_{k-1})\delta_{k-1}, & \text{by (4.6d)} \end{split}$$

and unraveling the recurrence yields (4.6b). Finally,

$$\begin{split} \ddot{z}_{k} &= \dot{s}_{k} - \dot{s}_{k-1} & \text{by (4.3)} \\ &= (s_{k} + \ddot{s}_{k})\sigma_{k} + \ddot{s}_{k} - \dot{s}_{k-1} & \text{by (4.4b)} \\ &= (s_{k} + \ddot{s}_{k})\sigma_{k} + \dot{y}_{k} & \text{by (4.3)} \\ &= (s_{k} + \ddot{s}_{k})\sigma_{k} + (x_{k} + \ddot{y}_{k})\eta_{k} + \ddot{y}_{k}. & \text{by (4.4a)} \end{split}$$

Recalling that $\eta_2 = 0$, it is straightforward to check (4.5) separately.

4.2 Second order deterministic bound

We present a second-order expression (Corollary 4.2) for the error in Algorithm 4.1, and discuss the discrepancy with several existing bounds (Remark 4.3).

The expressions below suggest that the errors in the 'correction' steps 3 and 5 of Algorithm 4.1 dominate the first order terms of the summation error.

Corollary 4.2 With assumptions (4.1), let $\mu_k \equiv \eta_k - \delta_k$, $2 \le k \le n-1$, and $\mu_n \equiv \eta_n$. Then the error in Algorithm 4.1 up to second order equals

$$e_{n} = \hat{s}_{n} - s_{n} = \dot{s}_{n} = s_{n}\sigma_{n} + (1 + \sigma_{n})\sum_{k=2}^{n} x_{k}\mu_{k} - \sum_{k=2}^{n-1} s_{k}\sigma_{k}(\mu_{k+1} + \beta_{k} + \delta_{k}) - \sum_{k=2}^{n-1} x_{k}\delta_{k}(\mu_{k+1} + \beta_{k} + \eta_{k}) + \mathcal{O}(u^{3}),$$

and the computed sum equals

$$\widehat{s}_n = \sum_{k=1}^n (1+\rho_k) x_k, \qquad |\rho_k| \le 3u + [4(n-k)+6]u^2 + \mathcal{O}(u^3).$$
(4.7)

Proof Truncate the expressions for \ddot{y}_k , \ddot{z}_k , and \ddot{c}_k to first order, and substitute them into (4.6b).

Remark 4.3 The error bounds for compensated summation have sometimes been misstated in the literature. In contrast to (4.7), the expressions in [8, Theorem 8], [10, (4.8)] and [20, Exercise 19 in Section 4.2.2] are equal to

$$\widehat{s}_n = \sum_{k=1}^n (1+\rho_k) x_k$$
 where $|\rho_k| \le 2u + \mathcal{O}(nu^2).$

It appears that this expression does not properly account for the final error σ_n . In comparison, [19, page 9-5] correctly states that

$$\widehat{s}_n + \widehat{c}_n = \sum_{k=1}^n (1 + \rho_k) x_k \quad \text{where} \quad |\rho_k| \le 2u + \mathcal{O}((n-k)u^2).$$

4.3 Probabilistic bounds

We derive probabilistic bounds for the child-errors in compensated summation (Lemma 4.4) and derive a bound on the summation error in terms of the child-error bounds (Theorem 4.5), which is, however, difficult to interpret. Thus, we express the child-error bounds mostly in terms of the partial sums (Lemma 4.6), which leads to an alternative probabilistic bound (Theorem 4.7).

We start with a probabilistic analogue of Lemma 2.8. The generic strategy would be to write each child-error in terms of a martingale involving the previous child-errors, and to bound them probabilistically with the Azuma-Hoeffding inequality (Lemma 1.2). Instead, we found it easier here to bound \ddot{s}_k Lemma 1.2, and then apply the triangle inequality to \ddot{y}_k , \ddot{z}_k , and \ddot{c}_k .

Lemma 4.4 Let $\sigma_2, \delta_2, \beta_2, \eta_3, \sigma_3, \delta_3, \ldots, \eta_n$ in (4.1), (4.2) and (4.3) be mean-independent zero-mean random variables, $0 < \eta < 1$, and $\lambda_{n,\eta} \equiv \sqrt{2 \ln(2n/\eta)}$. With probability at least $1 - \eta$, the following bounds hold simultaneously:

$$|\ddot{y}_k| \le Y_k, \qquad |\ddot{s}_k| \le S_k, \qquad |\ddot{z}_k| \le Z_k, \qquad |\ddot{c}_k| \le C_k, \qquad 2 \le k \le n,$$
(4.8)

where the quantities Y_k , S_k , Z_k , C_k are defined by

$$Y_2 \equiv 0, \qquad S_2 \equiv 0, \qquad Z_2 \equiv u|s_2|, \qquad C_2 \equiv u(|x_2| + Z_2) + u|s_2|, \qquad (4.9)$$

and ⁴ for $3 \le k \le n$,

$$Y_k \equiv C_{k-1}(1+u),$$
 (4.10a)

$$S_k \equiv \lambda_{n,\eta} u \left(\sum_{j=3}^k \left((|x_j| + Y_j)^2 + C_{j-1}^2 + (|x_{j-1}| + Z_{j-1})^2 \right) \right)^{1/2}, \qquad (4.10b)$$

$$Z_k \equiv u(|s_k| + S_k) + u(|x_k| + Y_k) + Y_k, \qquad (4.10c)$$

$$C_k \equiv u(|x_k| + Z_k) + u(|s_k| + S_k).$$
(4.10d)

Proof This is an induction proof over k and the failure probability η .

Induction basis k = 2 From (4.5) in Theorem 4.1 follows that (4.9) holds deterministically.

Induction hypothesis Assume that the bounds (4.8) hold simultaneously for $2 \le j \le k-1$ with probability at least $1 - (k-1)\eta/n$.

Induction step The induction hypothesis implies that $|\ddot{c}_{k-1}| \leq C_{k-1}$ holds with probability at least $1 - (k-1)\eta$. From (4.6a), it follows that

$$|\ddot{y}_k| = |\ddot{c}_{k-1}(1+\beta_{k-1})| \le C_{k-1}(1+u) = Y_k$$

always holds.

The expression (4.6b) for \ddot{s}_k can be written as a martingale with respect to $\sigma_2, \delta_2, \beta_2, \eta_3, \sigma_3, \delta_3, \ldots, \eta_k$. By the induction hypothesis, the bounds

$$|(x_j + \ddot{y}_j)\eta_j| \le u(|x_j| + Y_j), \qquad 3 \le j \le k$$
$$|\ddot{c}_{j-1}\beta_{j-1}| \le u C_{j-1},$$
$$|(x_{j-1} + \ddot{z}_{j-1})\delta_{j-1}| \le u(|x_{j-1}| + Z_{j-1})$$

all hold simultaneously with probability at least $1 - (k-1)\eta/n$. Lemma 1.2 then implies that $|\ddot{s}_k| \leq S_k$ holds with probability at least $1 - \eta/n$.

The bounds $|\ddot{z}_k| \leq Z_k$ and $|\ddot{c}_k| \leq C_k$ always hold, due to (4.6c) and (4.6d).

The following probabilistic bound expressed the error in compensated summation in terms of the bounds for child-errors.

Theorem 4.5 Let $\sigma_2, \delta_2, \beta_2, \eta_3, \ldots, \eta_n, \sigma_n$ in (4.1), (4.2) and (4.3) be mean-independent zero-mean random variables, $0 < \eta < 1$, $0 < \delta < 1 - \eta$, and $\lambda_{n,\eta} \equiv \sqrt{2 \ln(2n/\eta)}$. Then under (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 4.1 is bounded by

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left((s_n + S_n)^2 + \sum_{j=3}^n \left((|x_j| + Y_j)^2 + C_{j-1}^2 + (|x_{j-1}| + Z_{j-1})^2 \right) \right)^{1/2},$$

where Y_j , S_j , Z_j , C_j , $2 \le j \le n$, are defined in Lemma 4.4.

 $^4\,$ The bounds depend on n and $\eta,$ but we omit the subscripts, and simply write S_k instead of $S_{k,n,\eta}.$

Proof Keeping in mind that that $e_n = \dot{s}_n$, substitute (4.6b) into (4.4b), bound the magnitude of the summands with probability at least $1 - \eta$ via 4.4 and apply Lemma 1.3 with additional probability δ . This derivation mirrors the proof of Theorem 2.9 which relies on Lemma 2.8 to bound the magnitude of the summands in the martingale.

The significant number of interacting terms make Theorem 4.5 difficult to interpret, in comparison to Theorem 2.9. The simplest approach at this point would be to truncate the terms S_k, Y_k, Z_k, C_k so that the overall bound holds to second order (or higher, if desired). With Lemma 4.6 and Theorem 4.7, we instead show that it is possible to obtain a bound that holds to all orders, at the cost of a more complicated proof. Consequently we derive an alternative bound in the same manner as before, alternating between the triangle inequality and the following bound.

Lemma 4.6 There is a constant $\alpha = \sqrt{6} + O(u)$, so that the terms in Lemma 4.4 can be bounded by

$$\left(\sum_{j=3}^{k} \left(Y_j^2 + C_{j-1}^2 + Z_{j-1}^2\right)\right)^{1/2} \le \alpha u \left(\sum_{j=2}^{k-1} (|s_j| + |x_j| + S_j)^2\right)^{1/2}, \qquad 3 \le k \le n.$$

Proof The precise value of α is derived in the Appendix A.

The next bounds for compensated summation is expressed in terms of partial sums and inputs.

Theorem 4.7 Let $\sigma_2, \delta_2, \beta_2, \eta_3, \sigma_3, \delta_3, \ldots, \eta_n, \sigma_n$ be mean-independent zero-mean random variables, $0 < \eta < 1$, $0 < \delta < 1 - \eta$, and $\lambda_{n,\eta} \equiv \sqrt{2 \ln(2n/\eta)}$. Then with probability at least $1 - (\delta + \eta)$, the error in Algorithm 4.1 is bounded by

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(|s_n| + \gamma(\sqrt{2} + \alpha u)\sqrt{\sum_{k=2}^n x_k^2} + \gamma\alpha u\sqrt{\sum_{k=2}^n s_k^2} \right)$$
$$\le u\sqrt{2\ln(2/\delta)} \left(1 + \sqrt{2} + \sqrt{6}(\sqrt{n} + 1)u \right) \sum_{k=1}^n |x_k| + \mathcal{O}(u^3),$$

where

$$\alpha \equiv \frac{\sqrt{1+3(1+u)^2+2(1+u)^4}}{1-u(1+u)^2} = \sqrt{6} + \mathcal{O}(u),$$

$$\gamma \equiv \sqrt{1+\lambda_{n,\eta}^2 u^2} \left(1+\lambda_{n,\eta}\alpha\sqrt{2n}u^2 \exp\left(\lambda_{n,\eta}^2\alpha^2 nu^4\right)\right) = 1 + \mathcal{O}(u^2).$$

Proof Remember that $e_n = \dot{s}_n$, and abbreviate the summands in Theorem 4.5 and in (4.10b) by

$$R_j \equiv \left(\left(|x_j| + Y_j \right)^2 + C_{j-1}^2 + \left(|x_{j-1}| + Z_{j-1} \right)^2 \right)^{1/2}, \qquad 3 \le j \le n.$$

We treat $\sum_{j=3}^{n} R_j^2$ as a two-norm and apply the following inequality for non-negative vectors c, x, y, and z,

$$\left(\|x+y\|_{2}^{2}+\|x+z\|_{2}^{2}+\|c\|_{2}^{2}\right)^{1/2} \leq \sqrt{2}\|x\|_{2}+\|c+y+z\|_{2}$$

followed by Lemma 4.6, two triangle inequalities, and the definition of S_j ,

$$\begin{split} \left(\sum_{j=3}^{n} R_{j}^{2}\right)^{1/2} &\leq \sqrt{2} \left(\sum_{k=2}^{n} x_{k}^{2}\right)^{1/2} + \left(\sum_{j=3}^{n} \left(Y_{j}^{2} + C_{j-1}^{2} + Z_{j-1}^{2}\right)\right)^{1/2} \\ &\leq \sqrt{2} \left(\sum_{k=2}^{n} x_{k}^{2}\right)^{1/2} + \alpha u \left(\sum_{j=2}^{n-1} (|s_{j}| + |x_{j}| + S_{j})^{2}\right)^{1/2} \\ &\leq \sqrt{2} \left(\sum_{k=2}^{n} x_{k}^{2}\right)^{1/2} + \alpha u \left(\sum_{k=2}^{n} (|s_{k}| + |x_{k}|)^{2}\right)^{1/2} + \alpha u \left(\sum_{j=3}^{n-1} S_{j}^{2}\right)^{1/2} \\ &\leq (\sqrt{2} + \alpha u) \left(\sum_{k=2}^{n} x_{k}^{2}\right)^{1/2} + \alpha u \sqrt{\sum_{k=2}^{n} s_{k}^{2}} + \lambda \alpha u^{2} \left(\sum_{j$$

Proceed as in the proof of Theorem 2.12,

$$\left(\sum_{j=3}^{n} R_j^2\right)^{1/2} \le \left(\sum_{j=0}^{n} (\lambda_{n,\eta} \alpha u^2)^j \sqrt{\binom{n}{j}}\right) \left((\sqrt{2} + \alpha u) \sqrt{\sum_{k=2}^{n} x_k^2} + \alpha u \sqrt{\sum_{k=2}^{n} s_k^2}\right),\tag{4.11}$$

where

$$\sum_{j=1}^{n} (\lambda_{n,\eta} \alpha u^2)^j \sqrt{\binom{n}{j}} \le \lambda_{n,\eta} \alpha \sqrt{2n} u^2 \exp\left(\lambda_{n,\eta}^2 \alpha^2 n u^4\right).$$
(4.12)

From Theorem 4.5; the inequality $(a + b)^2 + c^2 \leq (a + \sqrt{b^2 + c^2})^2$ for $a, b, c \geq 0$; and the definition of S_n in (4.10b) follows

$$\begin{aligned} |\dot{s}_{n}| &\leq u\sqrt{2\ln(2/\delta)} \left((s_{n} + S_{n})^{2} + \sum_{j=3}^{n} R_{j}^{2} \right)^{1/2} \\ &\leq u\sqrt{2\ln(2/\delta)} |s_{n}| + u\sqrt{2\ln(2/\delta)} \left(S_{n}^{2} + \sum_{j=3}^{n} R_{j}^{2} \right)^{1/2} \\ &= u\sqrt{2\ln(2/\delta)} |s_{n}| + u\sqrt{2\ln(2/\delta)} \sqrt{1 + \lambda_{n,\eta}^{2} u^{2}} \left(\sum_{j=3}^{n} R_{j}^{2} \right)^{1/2}. \end{aligned}$$

Combine this with (4.11) and (4.12).

Note that γ remains close to 1 as long as $\lambda_{n,\eta} u \ll 1$ and $\lambda_{n,\eta} \alpha \sqrt{2n} u^2 \ll 1$.

5 Mixed precision

Mixed-precision algorithms aim to do as much of the computation as possible in a lower precision without significantly degrading the accuracy of the computed result; see the survey [1]. We extend Corollaries 2.10 and 2.14 to any number of precisions (Theorems 5.1 and 5.2), present the first probabilistic error bounds for the mixed precision FABsum algorithm (Corollary 5.3), and end with a heuristic for designing mixed-precision algorithms (Remark 5.4).

The FABsum summation algorithm [2, Algorithm 3.1] computes the sum $s_n = x_1 + \cdots + x_n$ in two stages. First, it splits the inputs into blocks of b numbers, and sums each block with a fast summation algorithm, say in low precision. Second, it sums the results with an accurate summation algorithm, say in high precision or with compensated summation. We extend our approach to mixed precision, and derive the first rigorous probabilistic error bounds for FABsum. Our computational model is very general, so that, in theory, each operation can be evaluated in a different precision.

Probabilistic model for sequences of roundoffs in mixed precision Extend model (1.2) for roundoffs in terms of mean-independent zero-mean random variables δ_k by assuming in addition that each δ_k can be a roundoff in a different precision u_k , that is, $|\delta_k| \leq u_k$, $1 \leq k \leq n$.

Below are the straightforward generalizations of Corollaries 2.10 and 2.14.

Theorem 5.1 Let $0 < \eta < 1$, $0 < \delta < 1 - \eta$, and $\lambda_{n,\eta} \equiv \sqrt{2 \ln(2n/\eta)}$. Then under (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 2.1 is bounded by

$$|e_n| \le \sqrt{2\ln(2/\delta)} \left(\sum_{j=2}^n u_j^2 (|s_j| + F_{j,n,\eta})^2 \right)^{1/2},$$
(5.1)

where $F_{j,n,\eta}$ are defined by the recurrence

$$F_{2,n,\eta} \equiv 0, \qquad F_{k,n,\eta} \equiv \lambda_{n,\eta} \left(\sum_{j \prec k} u_j^2 \left(|s_j| + F_{j,n,\eta} \right)^2 \right)^{1/2}, \qquad 3 \le k \le n.$$
(5.2)

We derive a closed-form error bound with the same techniques as in the proof of Theorem 2.12.

Theorem 5.2 Let $0 < \eta < 1$, and $0 < \delta < 1 - \eta$. Then under (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 2.1 is bounded by

$$\begin{aligned} |e_n| &\leq \sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,\tilde{h},\eta}\right) \sqrt{\sum_{k=2}^n u_k^2 s_k^2} \\ &\leq \sqrt{\tilde{h}} \sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,\tilde{h},\eta}\right) \sum_{k=1}^n |x_k|, \end{aligned}$$

where $\tilde{h} \equiv \max_k \sum_{k \prec \ell \prec n} u_\ell^2$ is the weighted height of the computational tree and

$$\phi_{n,\tilde{h},\eta} \equiv \lambda_{n,\eta} \sqrt{2\tilde{h}} u \exp\left(\lambda_{n,\eta}^2 \tilde{h} u^2\right) \qquad \text{with} \qquad \lambda_{n,\eta} \equiv \sqrt{2\ln(2n/\eta)}. \tag{5.3}$$

Proof Repeated application of the 2-norm triangle inequality implies that the bound

$$|e_n| \le \sqrt{2\ln(2/\delta)} \sum_{j=0}^h \lambda_{n,\eta}^j \left(\sum_{k=2}^n T_{k,j}^2 u_k^2 s_k^2 \right)^{1/2},$$
(5.4)

with

$$T_{k,0} \equiv 1, \qquad T_{k,j} \equiv \left(\sum_{k \prec \ell_1 \prec \dots \prec \ell_j \preceq n} (u_{\ell_1} \cdots u_{\ell_n})^2\right)^{1/2}, \qquad 2 \le k \le n, \qquad (5.5)$$

holds with probability at least $1 - (\delta + \eta)$. Now apply the Cauchy-Schwarz inequality (2.9) as before and swap the order of summation,

$$\sum_{j=1}^{h} \lambda_{n,\eta}^{j} \left(\sum_{k=2}^{n} T_{k,j}^{2} u_{k}^{2} s_{k}^{2} \right)^{1/2} \leq \left(\sum_{j=1}^{h} 2^{j} \lambda_{n,\eta}^{2j} \sum_{k=2}^{n} T_{k,j}^{2} u_{k}^{2} s_{k}^{2} \right)^{1/2} = \left(\sum_{k=2}^{n} \left(\sum_{j=1}^{h} 2^{j} \lambda_{n,\eta}^{2j} T_{k,j}^{2} \right) u_{k}^{2} s_{k}^{2} \right)^{1/2}.$$
(5.6)

With $\tilde{h}_k\equiv\sum_{k\prec\ell\preceq n}u_\ell^2$ being the weighted depth of node k, the inner sums are bounded by

$$\sum_{j=1}^{h} 2^{j} \lambda_{n,\eta}^{2j} T_{k,j}^{2} = \prod_{k \prec \ell \preceq n} (1 + 2\lambda_{n,\eta}^{2} u_{\ell}^{2}) - 1, \qquad 2 \le k \le n$$
$$\le \exp\left(2\lambda_{n,\eta}^{2} \tilde{h}_{k}\right) - 1 \le 2\lambda_{n,\eta}^{2} \tilde{h}_{k} \exp\left(2\lambda_{n,\eta}^{2} \tilde{h}_{k}\right),$$

Insert the bounds $\tilde{h}_k \leq \tilde{h}$ into (5.6),

$$\sum_{j=1}^{h} \lambda_{n,\eta}^{j} \left(\sum_{k=2}^{n} T_{k,j}^{2} u_{k}^{2} s_{k}^{2} \right)^{1/2} \leq \lambda_{n,\eta} \sqrt{2\tilde{h}} \exp\left(\lambda_{n,\eta}^{2} \tilde{h}\right) \sqrt{\sum_{k=2}^{n} u_{k}^{2} s_{k}^{2}},$$

and combine this inequality with (5.4).

As a corollary, we obtain the first rigorous probabilistic error bound for the mixed-precision version of FABsum [2] in Algorithm 5.1.

Algorithm 5.1 Mixed-precision FABsum Input: Floating point numbers x_1, \ldots, x_n ; block size b; precisions u_{lo}, u_{hi} Output: $s_n = \sum_{k=1}^n x_k$ 1: for k = 1 : n/b do 2: $s_k =$ output of Algorithm 2.1 applied to $x_{(k-1)b+1}, \ldots, x_{kb}$ in precision u_{lo} 3: end for

^{4:} s_n = output of Algorithm 2.1 applied to $s_1, \ldots, s_{n/b}$ in precision u_{hi}

Corollary 5.3 Let $0 < \eta < 1$; $0 < \delta < 1 - \eta$; h_{lo} the maximum height of all trees in the low-precision calls to Algorithm 2.1; h_{hi} the height of the portion of the tree in the high-precision call to Algorithm 2.1. Then under the mixed-precision extension of model (1.2), with probability at least $1 - (\delta + \eta)$, the error in Algorithm 5.1 is bounded by

$$|e_n| \le \sqrt{\tilde{h}} \sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,\tilde{h},\eta}\right) \sum_{k=1}^n |x_k|$$

where $\tilde{h} \equiv h_{lo}u_{lo}^2 + h_{hi}u_{hi}^2$, and $\phi_{n,\tilde{h},n}$ is defined in (5.3).

Remark 5.4 Inspired by the error expression in Theorem 5.2, we offer the following modified version of advice in Remark 2.5

In designing a mixed-precision summation method to achieve high accuracy, the aim should be to minimize the absolute values of the intermediate quantities $u_k s_k$.

The FABsum Algorithm 5.1 attempts to do just this by reserving its high-precision computations for the end, when the intermediate sums s_k are likely to have larger magnitudes.

6 Numerical experiments

After describing the setup, we present numerical experiments for recursive and pairwise summation (Section 6.1), shifted summation (Section 6.2), compensated summation (Section 6.3), and mixed-precision FABSum (Section 6.4).

Experiments are performed in MATLAB R2022a, with unit roundoffs [14]

- Half precision $u = 2^{-11} \approx 4.88 \cdot 10^{-4}$.
- Single precision $u_{\rm hi} = 2^{-24} \approx 5.96 \cdot 10^{-8}$ as the high precision in FABsum Algorithm 5.1.
- Double precision $u = 2^{-53} \approx 1.11 \cdot 10^{-16}$ for 'exact' computation.

Experiments plot errors from two rounding modes: round-to-nearest and stochastic rounding as implemented with chop [13].

The summands x_k are independent uniform [0, 1] random variables. The plots show relative errors $|\hat{s}_n - s_n|/|s_n|$ versus n, for $100 \le n \le 10^5$. We choose relative errors rather than absolute errors to allow for meaningful calibration: Relative errors $\le u$ indicate full accuracy; while relative errors $\ge .5$ indicate zero digits of accuracy.

For shifted summation we use the empirical mean of two extreme summands,

$$c = (\min_{k} x_k + \max_{k} x_k)/2.$$

For probabilistic bounds, the combined failure probability is $\delta + \eta = 10^{-2} + 10^{-3}$, hence $\sqrt{2\ln(2/\delta)} \approx 3.26$. For $n = 10^5$ and h = n we get $\lambda_{n,\eta} \approx 6.2$, and in half precision $u = 2^{-11}$ the higher-order errors, $1 + \phi_{n,h,\eta} \approx 4.4$, have a non-negligible effect on our bounds.

6.1 Sequential and pairwise summation

Figure 3 shows the errors in half precision from Algorithm 2.1 for sequential summation in one panel, and for pairwise summation in another panel, along with the deterministic bounds from Theorem 2.4,

$$|e_{n}| \leq \sum_{k=2}^{n} |s_{k}| |\delta_{k}| \prod_{k \prec j \leq n} |1 + \delta_{j}| \leq \lambda_{h} u \sum_{k=2}^{n} |s_{k}|$$
(6.1)

$$\leq \lambda_h h u \sum_{j=1}^n |x_j|. \tag{6.2}$$

and the probabilistic bounds from Corollary 2.14,

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,h,\eta}\right) \sqrt{\sum_{k=2}^n s_k^2}$$
 (6.3)

$$\leq u\sqrt{h}\sqrt{2\ln(2/\delta)}\left(1+\phi_{n,h,\eta}\right)\sum_{k=1}^{n}|x_{k}|,\tag{6.4}$$

Sequential summation The bound (6.3) remains within a factor of 2 of (6.4). Although the higher-order error terms $1 + \phi_{n,h,\eta}$ represent only a small part of the error bounds, they may still be pessimistic, as the bounds curve upwards for large n, while the actual errors increase more slowly. The reason may be the distribution of floating point numbers: spacing between consecutive numbers is constant within each interval $[2^t, 2^{t+1}]$, so a roundoff δ_k is affected by previous errors primarily if $\lfloor \log_2(\hat{s}_k) \rfloor \neq \lfloor \log_2(s_k) \rfloor$. Some analyses have derived deterministic error bounds for summation that do not contain second-order terms [16,17,21,25], and perhaps a more careful analysis will be able to do the same for probabilistic bounds. Our bounds otherwise accurately describe the behavior of stochastic rounding, but round-to-nearest suffers from stagnation for larger problem sizes.

Pairwise summation The bound (6.4) grows proportional to $\sqrt{\log_2(n)}$, while (6.3) remains essentially constant. The behavior of (6.3) may be due to the monotonically increasing partial sums for uniform [0, 1] inputs, where the final sum is likely to dominate all previous partial sums, $(\sum_{k=2}^{n} s_k^2)^{1/2} = \mathcal{O}(s_n)$. This suggests that pairwise summation of uniform [0, 1] inputs is highly accurate. The constant bound accurately describes the behavior of the error under stochastic rounding, but not round-to-nearest. We are not sure of the exact reason for the difference in behavior between the two.

6.2 Shifted summation

Figure 4 shows the errors in half precision from Algorithm 3.1 for shifted sequential summation and shifted pairwise summation, along with the probabilistic bounds



Fig. 3 Relative errors in half precision for recursive summation (left) and sequential summation (right) versus number of summands n. The symbol (+) indicates round-to-nearest (RTN), and (×) indicates stochastic rounding (SR). Horizontal line indicates unit roundoff $u = 2^{-11}$, and remaining points indicate deterministic bounds (6.1) and (6.2) and probabilistic bounds (6.3) and (6.4).



Fig. 4 Relative errors in half precision for shifted sequential summation (left) and shifted pairwise summation (right) versus number of summands n. The symbol (+) indicates round-to-nearest (RTN), and (×) indicates stochastic rounding (SR). Horizontal line indicates unit roundoff $u = 2^{-11}$, and remaining points indicate probabilistic bounds (6.5) and (6.6).

from Theorem 3.1,

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,h,\eta}\right) \sqrt{s_n^2 + \sum_{k=2}^n t_k^2 + \sum_{k=1}^{n+1} y_k^2}$$
(6.5)

$$\leq u\sqrt{2\ln(2/\delta)} \left(1+\phi_{n,h,\eta}\right) \left(n|c|+\sqrt{h}\sum_{k=1}^{n}\left(|x_k-c|+|x_k|\right)\right).$$
(6.6)

A comparison with Figure 3 shows that shifting reduces both the actual errors and the bounds. Errors are on the order of unit roundoff, in all cases: round-to-nearest and stochastic rounding, and sequential and pairwise summation.



Fig. 5 Relative errors in half precision for compensated summation (left) and mixed precision with FABsum with high precision $u_{\rm hi} = 2^{-24}$ (right) versus number of summands *n*. The symbol (+) indicates round-to-nearest (RTN), and (×) indicates stochastic rounding (SR). Horizontal line indicates unit roundoff $u_{\rm lo} = 2^{-11}$, and remaining points indicate bounds (6.7)-(6.10) (left) and (6.11)-(6.13) (right).

6.3 Compensated summation

The first panel in Figure 5 shows the errors in half precision for Algorithm 4.1 for $10^2 \leq n \leq 10^7$ summands⁵, along with deterministic bounds derived from Corollary 4.2,

$$|e_n| \le u|s_n| + 2u(1+3u) \sum_{k=2}^n |x_k| + 4u^2 \sum_{k=2}^{n-1} |s_k| + \mathcal{O}(u^3)$$
(6.7)

$$\leq (3u + (4n - 2)u^2) \sum_{k=1}^n |x_k| + \mathcal{O}(u^3), \tag{6.8}$$

and the probabilistic bounds from Theorem 4.7,

$$|e_n| \le u\sqrt{2\ln(2/\delta)} \left(|s_n| + \gamma(\sqrt{2} + \alpha u)\sqrt{\sum_{k=2}^n x_k^2} + \gamma \alpha u\sqrt{\sum_{k=2}^n s_k^2} \right) \tag{6.9}$$

$$\leq u\sqrt{2\ln(2/\delta)} \left(1 + \sqrt{2} + \sqrt{6}(\sqrt{n} + 1)u\right) \sum_{k=1}^{n} |x_k| + \mathcal{O}(u^3).$$
 (6.10)

The probabilistic bounds (6.9) and (6.10) track the error behavior accurately, with (6.9) even capturing the correct order of magnitude. This also illustrates the higher accuracy of bounds involving partial sums.

6.4 Mixed-precision FABsum summation

The second panel of Figure 5 shows the errors for Algorithm 5.1 with $u_{\rm lo} = 2^{-11} \approx 4.44 \cdot 10^{-4}$, $u_{\rm hi} = 2^{-24} \approx 5.96 \cdot 10^{-8}$, block size b = 32 and $10^2 \le n \le 10^7$ summands,

 $^{^5\,}$ Our simulation of half-precision ignores the range restriction ${\tt realmax}=65504.$

where each internal call to Algorithm 2.1 uses recursive summation. We also plot the deterministic first-order bound from [2, Eqn. 3.5],

$$|e_n| \le bu \sum_{k=1}^n |x_k| + \mathcal{O}(u^2),$$
 (6.11)

and the probabilistic bounds derived from Theorem 5.2,

$$|e_n| \le \sqrt{2\ln(2/\delta)} \left(1 + \phi_{n,\tilde{h},\eta}\right) \sqrt{\sum_{k=2}^n u_k^2 s_k^2}$$
(6.12)

$$\leq \sqrt{\tilde{h}}\sqrt{2\ln(2/\delta)} \left(1+\phi_{n,\tilde{h},\eta}\right) \sum_{k=1}^{n} |x_k|,\tag{6.13}$$

where $\tilde{h} = bu^2 + (n/b)u_{\rm hi}^2$. Errors are on the order of unit roundoff for round-tonearest. We were surprised to observe that for stochastic rounding, errors fell to more than an order of magnitude *below* unit roundoff for large problem sizes. This behavior is correctly predicted by the bound in terms of the partial sums (6.12) but not the bound in terms of the inputs (6.13), demonstrating the importance of error expressions involving the partial sums.

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A Proof of Lemma 4.6

Define $\beta \equiv u(1+u)^2$ and

$$\omega_k \equiv |s_k| + |x_k| + S_k, \qquad 2 \le k \le n - 1.$$
 (A.1)

Lemma 4.4 implies

$$Z_k = u\omega_k + (1+u)Y_k = u\omega_k + (1+u)^2C_{k-1}, \qquad 3 \le k \le n-1 \tag{A.2}$$

$$C_k = u\omega_k + uZ_k = u(1+u)\omega_k + \beta C_{k-1}, \tag{A.3}$$

where $Z_2 \leq u\omega_2$ and $C_2 \leq u(1+u)\omega_2$. For $3 \leq k \leq n$, define the vectors

$$\mathbf{c}_k \equiv \begin{bmatrix} C_{k-1} \cdots C_2 \end{bmatrix}^T, \quad \mathbf{z}_k \equiv \begin{bmatrix} Z_{k-1} \cdots Z_2 \end{bmatrix}^T, \quad \mathbf{w}_k \equiv \begin{bmatrix} \omega_{k-1} \cdots \omega_2 \end{bmatrix}^T.$$

From (A.3) follows the componentwise inequality

$$\mathbf{c}_k \le u(1+u)\mathbf{w}_k + \beta \mathbf{U}\mathbf{c}_k,$$

where U is an upper shift matrix. Solving for \mathbf{c}_k gives another componentwise inequality with a unit upper triangular matrix $\mathbf{I} - \beta \mathbf{U}$,

$$\mathbf{c}_k \leq u(1+u)(\mathbf{I}-\beta\mathbf{U})^{-1}\mathbf{w}_k$$

and a bound

$$\|\mathbf{c}_k\|_2 \le u(1+u)\|(\mathbf{I}-\beta\mathbf{U})^{-1}\mathbf{w}_k\|_2 \le \frac{u(1+u)}{1-\beta}\|\mathbf{w}_k\|_2.$$

The bound for $\|\mathbf{z}_k\|_2$ follows from (A.2) and the definition of β ,

$$\|\mathbf{z}_k\|_2 \le u \|\mathbf{w}_k\|_2 + (1+u)^2 \|\mathbf{c}_k\|_2 \le \frac{u(2+2u+u^2)}{1-\beta} \|\mathbf{w}_k\|_2.$$

Finally, from $Y_k = (1+u)C_{k-1}$ follows the Frobenius norm bound

$$\left(\sum_{j=3}^{k} \left(Y_{j}^{2} + C_{j-1}^{2} + Z_{j-1}^{2}\right)\right)^{1/2} = \left\|\left[(1+u)\mathbf{c}_{k} \ \mathbf{c}_{k} \ \mathbf{z}_{k}\right]\right\|_{F} \le \alpha u \|\mathbf{w}_{k}\|_{2},$$

where the higher order terms in α follow from the Taylor series expansion $(1 - \beta)^{-2} = 1 + 2u + O(u^2)$,

$$\alpha^2 = \frac{1+3(1+u)^2 + 2(1+u)^4}{(1-\beta)^2} = 6 + 26u + \mathcal{O}(u^2)$$

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