

ROUNDING ERROR ANALYSIS OF MIXED-PRECISION HOUSEHOLDER QR ALGORITHMS

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Abstract. Although mixed precision arithmetic has recently garnered interest for training dense neural networks, many other applications could benefit from the speed-ups and lower storage if applied appropriately. The growing interest in employing mixed precision computations motivates the need for rounding error analysis that properly handles behavior from mixed precision arithmetic. We present a framework for mixed precision analysis that builds on the foundations of rounding error analysis presented in [13] and demonstrate its practicality by applying the analysis to various Householder QR Algorithms.

1. Introduction. The accuracy of a numerical algorithm depends on several factors, including numerical stability and well-conditionedness of the problem, both of which may be sensitive to rounding errors, the difference between exact and finite-precision arithmetic. Low precision floats use fewer bits than high precision floats to represent the real numbers and naturally incur larger rounding errors. Therefore, error attributed to round-off may have a larger influence over the total error when using low precision, and some standard algorithms may yield insufficient accuracy when using low precision storage and arithmetic. However, many applications exist that would benefit from the use of lower precision arithmetic and storage that are less sensitive to floating-point round off error, such as clustering or ranking graph algorithms [21] or training dense neural networks [18], to name a few.

Many computing applications today require solutions quickly and often under low size, weight, and power constraints (low SWaP), e.g., sensor formation, etc. Computing in low-precision arithmetic offers the ability to solve many problems with improvement in all four parameters. Utilizing mixed-precision, one can achieve similar quality of computation as high-precision and still achieve speed, size, weight, and power constraint improvements. There have been several recent demonstrations of computing using half-precision arithmetic (16 bits) achieving around half an order to an order of magnitude improvement of these categories in comparison to double precision (64 bits). Trivially, the size and weight of memory required for a specific problem is $4\times$. Additionally, there exist demonstrations that the power consumption improvement is similar [9]. Modern accelerators (e.g., GPUs, Knights Landing, or Xeon Phi) are able to achieve this factor or better speedup improvements. Several examples include: (i) $2\text{--}4\times$ speedup in solving dense large linear equations [11, 12], (ii) $12\times$ speedup in training dense neural networks, and (iii) $1.2\text{--}10\times$ speedup in small batched dense matrix multiplication [1] (up to $26\times$ for batches of tiny matrices). Training deep artificial neural networks by employing lower precision arithmetic to various tasks such as multiplication [5] and storage [6] can easily be implemented on GPUs and are already a common practice in data science applications.

The low precision computing environments that we consider are *mixed precision* settings, which are designed to imitate those of new GPUs that employ multiple precision types for certain tasks. For example, Tesla V100's Tensor Cores perform matrix-multiply-and-accumulate of half precision input data with exact products and single precision (32 bits) summation accumulate [3]. The existing rounding error analyses are built within what we call a *uniform precision* setting, which is the assumption that all arithmetic operations and storage are performed via the same precision. In

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42 this work, we develop a framework for deterministic mixed-precision rounding error analysis, and
 43 explore half-precision Householder QR factorization (HQR) algorithms for data and graph analysis
 44 applications. QR factorization is known to provide a backward stable solution to the linear least
 45 squares problem and thus, is ideal for mixed-precision.

46 However, additional analysis is needed as the additional round-off error will effect orthogonality,
 47 and thus the accuracy of the solution. Here, we focus on analyzing specific algorithms in a specific
 48 set of types (IEEE754 half (fp16), single (fp32, and double(fp64)), but the framework we develop
 49 could be used on different algorithms or different floating point types (such as bfloat16 in [20]).

50 This work discusses several aspects of using mixed-precision arithmetic: (i) error analysis that
 51 can more accurately describe mixed-precision arithmetic than existing analyses, (ii) algorithmic de-
 52 sign that is more resistant against lower numerical stability associated with lower precision types,
 53 and (iii) an example where mixed-precision implementation performs as sufficiently as double-
 54 precision implementations. Our key findings are that the new mixed-precision error analysis pro-
 55 duces tighter error bounds, that some block QR algorithms by Demmel et al. [8] are able to operate
 56 in low precision more robustly than non-block techniques, and that some small-scale benchmark
 57 graph clustering problems can be successfully solved with mixed-precision arithmetic.

2. Background: Build up to rounding error analysis for inner products. In this
 section, we introduce the basic motivations and tools for mixed-precision rounding error analysis
 needed for the *QR factorization*. A matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ for $m \geq n$ can be written as

$$\mathbf{A} = \mathbf{Q}\mathbf{R}, \quad \mathbf{Q} \in \mathbb{R}^{m \times m}, \quad \mathbf{R} \in \mathbb{R}^{m \times n},$$

58 where \mathbf{Q} is orthogonal, $\mathbf{Q}^\top \mathbf{Q} = \mathbf{I}_{m \times m}$, and \mathbf{R} is upper trapezoidal. The above formulation is a
 59 *full* QR factorization, whereas a more efficient *thin* QR factorization results in $\mathbf{Q}_1 \in \mathbb{R}^{m \times n}$ and
 60 $\mathbf{R}_1 \in \mathbb{R}^{n \times n}$, that is

$$61 \quad \mathbf{A} = \mathbf{Q}\mathbf{R} = [\mathbf{Q}_1 \quad \mathbf{Q}_2] \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{0}_{m-n \times n} \end{bmatrix} = \mathbf{Q}_1 \mathbf{R}_1.$$

62 If \mathbf{A} is full rank then the columns of \mathbf{Q}_1 are orthonormal (i.e. $\mathbf{Q}_1^\top \mathbf{Q}_1 = \mathbf{I}_{n \times n}$) and \mathbf{R}_1 is upper
 63 triangular. In many applications, computing the *thin* decomposition requires less computation and
 64 is sufficient in performance. While important definitions are stated explicitly in the text, Table 1
 65 serves to establish basic notation.

Symbol(s)	Definition(s)	Section(s)
\mathbf{x}, \mathbf{A}	Vector, matrix	2
\mathbf{Q}	Orthogonal factor $\mathbf{A} \in \mathbb{R}^{m \times n}$: m -by- m (full) or m -by- n (thin)	2
\mathbf{R}	Upper triangular or trapezoidal factor of $\mathbf{A} \in \mathbb{R}^{m \times n}$: m -by- n (full) or n -by- n (thin)	2
$\text{fl}(\mathbf{x}), \hat{\mathbf{x}}$	Quantity \mathbf{x} calculated from floating point operations	2.1
b, t, μ, η	Base/precision/mantissa/exponent bits	2.1
k	Number of successive FLOPs	2.1
u^q	Unit round-off for precision t_q and base b_q : $\frac{1}{2}b_q^{1-t_q}$	2.1
δ^q	Quantity bounded by: $ \delta^q < u^q$	2.1
γ_k^q, θ_k^q	$\frac{ku^q}{1-ku^q}$, Quantity bounded by: $ \theta_k^q \leq \gamma_k^q$	2.1

TABLE 1
Basic definitions

Subsection 2.1 introduces basic concepts for rounding error analysis, and Subsection 2.2 exemplifies the need for mixed-precision rounding error analysis using the inner product.

2.1. Basic rounding error analysis of floating point operations. We use and analyze the IEEE 754 Standard floating point number systems. Let $\mathbb{F} \subset \mathbb{R}$ denote the space of some floating point number system with base $b \in \mathbb{N}$, precision $t \in \mathbb{N}$, significand $\mu \in \mathbb{N}$, and exponent range $[\eta_{\min}, \eta_{\max}] \subset \mathbb{Z}$. Then every element y in \mathbb{F} can be written as

$$(2.1) \quad y = \pm \mu \times b^{\eta-t},$$

where μ is any integer in $[0, b^t - 1]$ and η is an integer in $[\eta_{\min}, \eta_{\max}]$. While base, precision, and exponent range are fixed and define a floating point number, the sign, significand, and exponent identifies a unique number within that system. Although operations we use on \mathbb{R} cannot be replicated exactly due to the finite cardinality of \mathbb{F} , we can still approximate the accuracy of analogous floating point operations (FLOPs). We adopt the rounding error analysis tools described in [13], which allow a relatively simple framework for formulating error bounds for complex linear algebra operations. A short analysis of FLOPs (see Theorem 2.2 [13]) shows that the relative error is controlled by the unit round-off, $u := \frac{1}{2}b^{1-t}$.

Name	b	t	# of exponent bits	η_{\min}	η_{\max}	unit round-off u
fp16 (IEEE754 half)	2	11	5	-15	16	4.883e-04
fp32 (IEEE754 single)	2	24	8	-127	128	5.960e-08
fp64 (IEEE754 double)	2	53	11	-1023	1024	1.110e-16

TABLE 2
IEEE754 formats and their primary attributes.

Let ‘op’ be any basic operation from the set $\text{OP} = \{+, -, \times, \div\}$ and let $x, y \in \mathbb{R}$. The true value $(x \text{ op } y)$ lies in \mathbb{R} , and it is rounded using some conversion to a floating point number, $\text{fl}(x \text{ op } y)$, admitting a rounding error. The IEEE 754 Standard requires *correct rounding*, which rounds the exact solution $(x \text{ op } y)$ to the closest floating point number and, in case of a tie, to the floating point number that has a mantissa ending in an even number. *Correct rounding* gives us an assumption for the error model where a single basic floating point operation yields a relative error, δ , bounded in the following sense:

$$(2.2) \quad \text{fl}(x \text{ op } y) = (1 + \delta)(x \text{ op } y), \quad |\delta| \leq u, \quad \text{op} \in \{+, -, \times, \div\}.$$

We use (2.2) as a building block in accumulating errors from successive FLOPs. For example, consider computing $x + y + z$, where $x, y, z \in \mathbb{R}$ with a machine that can only compute one operation at a time. Then, there is a rounding error in computing $\hat{s}_1 := \text{fl}(x + y) = (1 + \delta)(x + y)$, and another rounding error in computing $\hat{s}_2 := \text{fl}(\hat{s}_1 + z) = (1 + \tilde{\delta})(\hat{s}_1 + z)$, where $|\delta|, |\tilde{\delta}| < u$. Then,

$$(2.3) \quad \text{fl}(x + y + z) = (1 + \tilde{\delta})(1 + \delta)(x + y) + (1 + \tilde{\delta})z.$$

Multiple successive operations introduce multiple rounding error terms, and keeping track of all errors is challenging. Lemma 2.1 introduces a convenient and elegant bound that simplifies accumulation of rounding error.

97 LEMMA 2.1 (Lemma 3.1 [13]). Let $|\delta_i| < u$ and $\rho_i \in \{-1, +1\}$, for $i = 1, \dots, k$ and $ku < 1$.
 98 Then,

$$99 \quad (2.4) \quad \prod_{i=1}^k (1 + \delta_i)^{\rho_i} = 1 + \theta_k, \quad \text{where} \quad |\theta_k| \leq \frac{ku}{1 - ku} =: \gamma_k.$$

100 We also use

$$101 \quad \tilde{\gamma}_k = \frac{cku}{1 - cku},$$

102 where $c > 0$ is a small integer and further extend this to θ so that $|\tilde{\theta}_k| \leq \tilde{\gamma}_k$.

103 In other words, θ_k represents the accumulation of rounding errors from k successive operations, and
 104 it is bounded by γ_k . Allowing θ_k 's to be any arbitrary value within the corresponding γ_k bounds
 105 further aids in keeping a clear, simple error analysis. Applying this lemma to our example of adding
 106 three numbers results in

$$107 \quad (2.5) \quad \text{fl}(x + y + z) = (1 + \tilde{\delta})(1 + \delta)(x + y) + (1 + \tilde{\delta})z = (1 + \theta_2)(x + y) + (1 + \theta_1)z.$$

108 Since $|\theta_1| \leq \gamma_1 < \gamma_2$, we can further simplify (2.5) to

$$109 \quad (2.6) \quad \text{fl}(x + y + z) = (1 + \tilde{\theta}_2)(x + y + z), \quad \text{where} \quad |\tilde{\theta}_2| \leq \gamma_2,$$

110 at the cost of a slightly larger upper bound. Typically, error bounds formed in the fashion of (2.6)
 111 are converted to relative errors in order to put the error magnitudes in perspective. The relative
 112 error bound for our example is

$$113 \quad \frac{|(x + y + z) - \text{fl}(x + y + z)|}{|x + y + z|} \leq \gamma_2$$

114 when we assume $x + y + z \neq 0$.

115 Although Lemma 2.1 requires $ku < 1$, we actually need $ku < \frac{1}{2}$ to maintain a meaningful
 116 relative error bound as this assumption implies $\gamma_k < 1$ and guarantees a relative error below 100%.
 117 Since higher precision floating points have smaller unit round-off values, they can tolerate more
 118 successive FLOPs than lower precision floating points before reaching $\gamma_m = 1$. Table 3 shows the
 119 maximum number of successive floating point operations that still guarantees a relative error below
 100% for various floating point types. Thus, accumulated rounding errors in lower precision types

precision	$\tilde{k} = \arg \max_k (\gamma_k \leq 1)$
FP16	512
FP32	$\approx 4.194\text{e}06$
FP64	$\approx 2.252\text{e}15$

TABLE 3
Upper limits of meaningful relative error bounds in the $\gamma^{(k)}$ notation.

120 can lead to an instability with fewer operations in comparison to higher precision types and prompts
 122 us to evaluate whether existing algorithms can be naively adapted for mixed-precision arithmetic.

2.2. Rounding Error Example for the Inner Product. We now consider computing the inner product of two vectors to clearly illustrate how this situation restricts rounding error analysis in fp16. An error bound for an inner product of m -length vectors is

$$(2.7) \quad |\mathbf{x}^\top \mathbf{y} - \text{fl}(\mathbf{x}^\top \mathbf{y})| \leq \gamma_m |\mathbf{x}|^\top |\mathbf{y}|, \quad \mathbf{x}, \mathbf{y} \in \mathbb{R}^m$$

as shown in [13]. While this result does not guarantee a high relative accuracy when $|\mathbf{x}^\top \mathbf{y}| \ll |\mathbf{x}|^\top |\mathbf{y}|$, high relative accuracy is expected in some special cases. For example, let $\mathbf{x} = \mathbf{y}$. Then we have exactly $|\mathbf{x}^\top \mathbf{x}| = |\mathbf{x}|^\top |\mathbf{x}| = \|\mathbf{x}\|_2^2$, which leads to a forward error: $|\|\mathbf{x}\|_2^2 - \text{fl}(\|\mathbf{x}\|_2^2)| \leq \gamma_m \|\mathbf{x}\|_2^2$. Since vectors of length m accumulate rounding errors that are bounded by γ_m , the dot products of vectors computed in fp16 already face a 100% relative error bound in the worst-case scenario ($\gamma_{512}^{\text{fp16}} = 1$).

We present a simple numerical experiment that shows that the standard deterministic error bound is too pessimistic and cannot be practically used to approximate rounding error for half-precision arithmetic. In this experiment, we generated 2 million random half-precision vectors of length 512 from two random distributions: the standard normal distribution, $N(0,1)$, and the uniform distribution over $(0,1)$. Half precision arithmetic was simulated by calling `alg. 1`, which was proven to be a faithful simulation in [15], for every FLOP (multiplication and addition for the dot product). The relative error in this experiment is formulated as the LHS in Equation 2.7 divided by $|\mathbf{x}|^\top |\mathbf{y}|$ and all operations outside of calculating $\text{fl}(\mathbf{x}^\top \mathbf{y})$ are executed by casting up to fp64 and using fp64 arithmetic. Table 4 shows some statistics from computing the relative error for simulated half precision dot products of 512-length random vectors. We see that the inner products of vectors sampled from the standard normal distribution have backward relative errors that do not deviate much from the unit round-off ($\mathcal{O}(1\text{e-}4)$), whereas the vectors sampled from the uniform distribution tend to accumulate larger errors on average ($\mathcal{O}(1\text{e-}3)$). Even so, the theoretical upper error bound of 100% is far too pessimistic as the maximum relative error does not even meet 2% in this experiment. Recent work in developing probabilistic bounds on rounding errors of floating point operations (see [14, 17]) have shown that the inner product relative backward error for the conditions used for this experiment is bounded by $5.466\text{e-}2$ with probability 0.99.

Algorithm 1: $\mathbf{z}^{\text{fp16}} = \text{simHalf}(f, \mathbf{x}^{\text{fp16}}, \mathbf{y}^{\text{fp16}})$. Simulate function $f \in \text{OP} \cup \{\text{dot_product}\}$ in half precision arithmetic given input variables \mathbf{x}, \mathbf{y} . Function `castup` converts half precision floats to single precision floats, and `castdown` converts single precision floats to half precision floats by rounding to the nearest half precision float.

Input: $\mathbf{x}^{\text{fp16}}, \mathbf{y}^{\text{fp16}} \in \mathbb{F}_{\text{fp16}}^m, f : \mathbb{R}^m \times \mathbb{R}^m \rightarrow \mathbb{R}^n$

Output: $\text{fl}(f(\mathbf{x}^{\text{fp16}}, \mathbf{y}^{\text{fp16}})) \in \mathbb{F}_{\text{fp16}}^n$

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1  $\mathbf{x}^{\text{fp32}}, \mathbf{y}^{\text{fp32}} \leftarrow \text{castup}([\mathbf{x}^{\text{fp16}}, \mathbf{y}^{\text{fp16}}])$ 
2  $\mathbf{z}^{\text{fp32}} \leftarrow \text{fl}(f(\mathbf{x}^{\text{fp32}}, \mathbf{y}^{\text{fp32}}))$ 
3  $\mathbf{z}^{\text{fp16}} \leftarrow \text{castdown}(\mathbf{z}^{\text{fp32}})$ 
4 return  $\mathbf{z}^{\text{fp16}}$ 
```

Most importantly, no rounding error bounds (deterministic or probabilistic) allow flexibility in the precision types used for different operations. This restriction is the biggest obstacle in gaining an understanding of rounding errors to expect from computations done on emerging hardware that support mixed-precision such as GPUs that employ mixed-precision arithmetic.

Random Distribution	Average	Standard deviation	Maximum
Standard normal	1.627e-04	1.640e-04	2.838e-03
Uniform (0, 1)	2.599e-03	1.854e-03	1.399e-02

TABLE 4

Statistics from dot product backward relative error in for 512-length vectors stored in half-precision and computed in simulated half-precision from 2 million realizations.

We start by introducing some additional rules from [13] that build on Lemma 2.1 in Lemma 2.2. These rules summarize how to accumulate errors represented by θ 's and γ 's in a *uniform precision* setting. These relations aid in writing clear and simpler error analyses. Regardless of the specific details of a mixed-precision setting, a rounding error analysis for mixed-precision arithmetic must support at least two different precision types. Thus, Lemma 2.3 allows low and high precision types and is a simple modification of Lemma 2.2. The rules for θ allows us to keep track of the two precision types separately and the rules we present for γ were chosen to be useful for casting down to the lower of the two precisions, a pertinent procedure in our mixed-precision analysis in the later sections.

LEMMA 2.2. For any positive integer k , let θ_k denote a quantity bounded according to $|\theta_k| \leq \frac{ku}{1-ku} =: \gamma_k$. The following relations hold for positive integers i, j , and nonnegative integer k . Arithmetic operations between θ_k 's:

$$(2.8) \quad (1 + \theta_k)(1 + \theta_j) = (1 + \theta_{k+j}) \quad \text{and} \quad \frac{1 + \theta_k}{1 + \theta_j} = \begin{cases} 1 + \theta_{k+j}, & j \leq k \\ 1 + \theta_{k+2j}, & j > k \end{cases}$$

Operations on γ 's:

$$\begin{aligned} \gamma_k \gamma_j &\leq \gamma_{\min(k,j)}, \quad \text{for } \max_{(j,k)} u \leq \frac{1}{2}, \\ n\gamma_k &\leq \gamma_{nk}, \quad \text{for } n \leq \frac{1}{uk}, \\ \gamma_k + u &\leq \gamma_{k+1}, \\ \gamma_k + \gamma_j + \gamma_k \gamma_j &\leq \gamma_{k+j}. \end{aligned}$$

LEMMA 2.3. For any nonnegative integer k and some precision q , let θ_k^q denote a quantity bounded according to $|\theta_k^q| \leq \frac{ku^q}{1-ku^q} =: \gamma_k^q$. The following relations hold for two precisions l (low) and h (high), positive integers j_l, j_h , non-negative integers k_l , and k_h , and $c > 0$:

$$(2.9) \quad (1 + \theta_{k_l}^l)(1 + \theta_{j_l}^l)(1 + \theta_{k_h}^h)(1 + \theta_{j_h}^h) = (1 + \theta_{k_l+j_l}^l)(1 + \theta_{k_h+j_h}^h),$$

$$(2.10) \quad \frac{(1 + \theta_{k_l}^l)(1 + \theta_{j_l}^l)}{(1 + \theta_{j_l}^l)(1 + \theta_{j_h}^h)} = \begin{cases} (1 + \theta_{k_h+j_h}^h)(1 + \theta_{k_l+j_l}^l), & j_h \leq k_h, j_l \leq k_l, \\ (1 + \theta_{k_h+2j_h}^h)(1 + \theta_{k_l+j_l}^l), & j_h \leq k_h, j_l > k_l, \\ (1 + \theta_{k_h+j_h}^h)(1 + \theta_{k_l+2j_l}^l), & j_h > k_h, j_l \leq k_l, \\ (1 + \theta_{k_h+2j_h}^h)(1 + \theta_{k_l+2j_l}^l), & j_h > k_h, j_l > k_l. \end{cases}$$

Without loss of generality, let $1 \gg u_l \gg u_h > 0$. Let d , a nonnegative integer, and $r \in [0, \lfloor \frac{u_l}{u_h} \rfloor]$ be numbers that satisfy $k_h u_h = d u_l + r u_h$. Alternatively, d can be defined by $d := \lfloor \frac{k_h u_h}{u_l} \rfloor$. Then,

$$(2.11) \quad \gamma_{k_h}^h \gamma_{k_l}^l \leq \gamma_{k_l}^l, \quad \text{for } k_l u^l \leq \frac{1}{2}$$

$$(2.12) \quad \gamma_{k_h}^h + u^l \leq \gamma_{d+2}^l$$

$$(2.13) \quad \gamma_{k_l}^l + u^h \leq \gamma_{k_l+1}^l$$

$$(2.14) \quad \gamma_{k_l}^l + \gamma_{k_h}^h + \gamma_{k_l}^l \gamma_{k_h}^h < \gamma_{k_l+d+1}^l.$$

We use these principles to establish a mixed-precision rounding error analysis for computing the dot product, which is crucial in many linear algebra routines such as the QR factorization. Let us define an ad hoc mixed-precision setting that is similar to the TensorCore Fused Multiply-Add (FMA) block but works at the level of a dot product. While the FMA block in TensorCore is for matrix-matrix products (level-3 BLAS), we consider a vector inner product (level-2 BLAS) FMA as defined in Assumption 2.4.

ASSUMPTION 2.4. Let l and h each denote low and high precision types with unit round-off values u^l and u^h , where $1 \gg u^l \gg u^h > 0$. Consider an FMA operation for inner products that take vectors stored in precision l , compute products in full precision, and sum the products in precision h . Finally, the result is then cast back down to precision l .

The full precision multiplication in Assumption 2.4 is exact when the low precision type is fp16 and the high precision type of fp32 due to their specifications for precision and exponent range. As a quick proof, consider $x^{\text{fp16}} = \pm \mu_x 2^{\eta_x - 11}$, $y^{\text{fp16}} = \pm \mu_y 2^{\eta_y - 11}$ where $\mu_x, \mu_y \in [0, 2^{11} - 1]$ and $\eta_x, \eta_y \in [-15, 16]$. Then the product in exact arithmetic is

$$x^{\text{fp16}} y^{\text{fp16}} = \pm \mu_x \mu_y 2^{\eta_x + \eta_y + 2 - 24},$$

where $\mu_x \mu_y \in [0, (2^{11} - 1)^2] \subseteq [0, 2^{24} - 1]$ and $\eta_x + \eta_y + 2 \in [-28, 34] \subseteq [-127, 128]$. Thus, the summation and the final cast down operations are the only sources of rounding error.

Let $\mathbf{x}^{\text{fp16}}, \mathbf{y}^{\text{fp16}}$ be m -length vectors stored in fp16, s_k be the k^{th} partial sum, and \hat{s}_k be s_k computed with FLOPs. Then,

$$\begin{aligned} \hat{s}_1 &= \text{fl}(\mathbf{x}_1 \mathbf{y}_1) = \mathbf{x}_1 \mathbf{y}_1, \\ \hat{s}_2 &= \text{fl}(\hat{s}_1 + \mathbf{x}_2 \mathbf{y}_2) = (\mathbf{x}_1 \mathbf{y}_1 + \mathbf{x}_2 \mathbf{y}_2) (1 + \delta_1^h), \\ \hat{s}_3 &= \text{fl}(\hat{s}_2 + \mathbf{x}_3 \mathbf{y}_3) = [(\mathbf{x}_1 \mathbf{y}_1 + \mathbf{x}_2 \mathbf{y}_2) (1 + \delta_1^h) + \mathbf{x}_3 \mathbf{y}_3] (1 + \delta_2^h). \end{aligned}$$

We can see a pattern emerging. The error for a general m -length vector dot product is then

$$(2.15) \quad \hat{s}_m = (\mathbf{x}_1 \mathbf{y}_1 + \mathbf{x}_2 \mathbf{y}_2) \prod_{k=1}^{m-1} (1 + \delta_k^h) + \sum_{i=3}^n \mathbf{x}_i \mathbf{y}_i \left(\prod_{k=i-1}^{m-1} (1 + \delta_k^h) \right).$$

Using Lemma 2.1, we further simplify and form componentwise backward errors with

$$(2.16) \quad \text{fl}(\mathbf{x}^\top \mathbf{y}) = (\mathbf{x} + \Delta \mathbf{x})^\top \mathbf{y} = \mathbf{x}^\top (\mathbf{y} + \Delta \mathbf{y}), \quad \text{for } |\Delta \mathbf{x}| \leq \gamma_{m-1}^h |\mathbf{x}|, \quad |\Delta \mathbf{y}| \leq \gamma_{m-1}^h |\mathbf{y}|.$$

Casting this down to fp16, then we incur a rounding error quantified by $d := \lfloor \frac{(m-1)u^h}{u^l} \rfloor$. The resulting componentwise backward errors are

$$(2.17) \quad \text{fl}(\mathbf{x}^\top \mathbf{y}) = (\mathbf{x} + \Delta \mathbf{x})^\top \mathbf{y} = \mathbf{x}^\top (\mathbf{y} + \Delta \mathbf{y}), \quad \text{for } |\Delta \mathbf{x}| \leq \gamma_{d+1}^l |\mathbf{x}|, \quad |\Delta \mathbf{y}| \leq \gamma_{d+1}^l |\mathbf{y}|.$$

Equations (2.16) and (2.17) are crucial for our analysis in section 4 since the TensorCore technology outputs a matrix product in fp16 or fp32. Consider matrices $\mathbf{A} \in \mathbb{F}_{\text{fp16}}^{p \times m}$ and $\mathbf{B} \in \mathbb{F}_{\text{fp16}}^{m \times q}$, and $\mathbf{D} = \mathbf{AB} \in \mathbb{F}_{\text{fp16}}^{p \times q}$. If $\text{fl}(\mathbf{D})$ is desired in fp16, then each component of that matrix incurs rounding errors as shown in (2.17) and if it is desired in fp32, the componentwise rounding error is given by (2.16). Similarly, we could consider other mixed-precision algorithms that cast down at various points within the algorithm to take advantage of better storage properties of lower precision types. Error bounds in the fashion of (2.16) can be used before the cast down operations, and the action of the cast down is best represented by error bounds similar to (2.17).

In section 3, we introduce various Householder QR algorithms as well as a skeleton for rounding error analysis for these algorithms that we will modify for different mixed precision assumptions in section 4.

3. Algorithms and existing round-off error analyses. We introduce the Householder QR factorization algorithm (HQR) in subsection 3.1 and two block variants that use HQR within the block in subsections 3.2 and 3.3. The blocked HQR (BQR) in subsection 3.2 partitions the columns of the target matrix and utilizes mainly level-3 BLAS operations and is a well-known algorithm that uses the WY representation of [4]. In contrast, the Tall-and-Skinny QR (TSQR) in subsection 3.3 partitions rows of the matrix and takes a communication-avoiding divide-and-conquer approach that can be easily parallelized (see [7]). We also present the crucial results in standard rounding error analysis of these algorithms that excludes any mixed-precision assumptions. These building steps of round-off error analysis will be easily tweaked for various mixed-precision assumptions in section 4.

3.1. Householder QR (HQR). The HQR algorithm uses Householder transformations to zero out elements below the diagonal of a matrix (see [16]). We present this as zeroing out all but the first element of some vector, $\mathbf{x} \in \mathbb{R}^m$.

LEMMA 3.1. *Given vector $\mathbf{x} \in \mathbb{R}^m$, there exist Householder vector, \mathbf{v} , and Householder transformation matrix, $\mathbf{P}_{\mathbf{v}}$, such that $\mathbf{P}_{\mathbf{v}}$ zeros out \mathbf{x} below the first element.*

$$(3.1) \quad \begin{aligned} \sigma &= -\text{sign}(\mathbf{x}_1) \|\mathbf{x}\|_2, \quad \mathbf{v} = \mathbf{x} - \sigma \hat{\mathbf{e}}_1, \\ \beta &= \frac{2}{\mathbf{v}^\top \mathbf{v}} = -\frac{1}{\sigma \mathbf{v}_1}, \quad \mathbf{P}_{\mathbf{v}} = \mathbf{I}_m - \beta \mathbf{v} \mathbf{v}^\top. \end{aligned}$$

The transformed vector, $\mathbf{P}_{\mathbf{v}} \mathbf{x}$, has the same 2-norm as \mathbf{x} since Householder transformations are orthogonal: $\mathbf{P}_{\mathbf{v}} \mathbf{x} = \sigma \hat{\mathbf{e}}_1$. In addition, $\mathbf{P}_{\mathbf{v}}$ is symmetric and orthogonal, $\mathbf{P}_{\mathbf{v}} = \mathbf{P}_{\mathbf{v}}^\top = \mathbf{P}_{\mathbf{v}}^{-1}$.

3.1.1. HQR: Algorithm. Given $\mathbf{A} \in \mathbb{R}^{m \times n}$ and Lemma 3.1, HQR is done by repeating the following processes until only an upper triangle matrix remains. For $i = 1, 2, \dots, n$,
Step 1) Compute \mathbf{v} and β that zeros out the i^{th} column of \mathbf{A} beneath a_{ii} (see alg. 2), and
Step 2) Apply $\mathbf{P}_{\mathbf{v}}$ to the bottom right partition, $\mathbf{A}[i : m, i : n]$ (lines 4-6 of alg. 3).

Consider the following 4-by-3 matrix example adapted from [13]. Let \mathbf{P}_i represent the i^{th} Householder transformation of this algorithm.

$$\mathbf{A} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \xrightarrow{\text{apply } \mathbf{P}_1 \text{ to } \mathbf{A}} \left[\begin{array}{c|cc} \times & \times & \times \\ \hline 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{array} \right] \xrightarrow{\text{apply } \mathbf{P}_2 \text{ to } \mathbf{P}_1 \mathbf{A}}$$

248

249

$$\left[\begin{array}{cc|c} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{array} \right] \xrightarrow{\text{apply } \mathbf{P}_3 \text{ to } \mathbf{P}_2 \mathbf{P}_1 \mathbf{A}} \left[\begin{array}{ccc} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{array} \right] = \mathbf{P}_3 \mathbf{P}_2 \mathbf{P}_1 \mathbf{A} =: \mathbf{R}$$

250 Then, the \mathbf{Q} factor for a full QR factorization is $\mathbf{Q} := \mathbf{P}_1 \mathbf{P}_2 \mathbf{P}_3$ since \mathbf{P}_i 's are symmetric, and the
 251 thin factors for a general matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ are

$$252 \quad (3.2) \quad \mathbf{Q}_{\text{thin}} = \mathbf{P}_1 \cdots \mathbf{P}_n \mathbf{I}_{m \times n} \quad \text{and} \quad \mathbf{R}_{\text{thin}} = \mathbf{I}_{m \times n}^\top \mathbf{P}_n \cdots \mathbf{P}_1 \mathbf{A}.$$

Algorithm 2: $\beta, \mathbf{v}, \sigma = \text{hh_vec}(\mathbf{x})$. Given a vector $\mathbf{x} \in \mathbb{R}^n$, return $\mathbf{v}, \beta, \sigma$ that satisfy $(I - \beta \mathbf{v} \mathbf{v}^\top) \mathbf{x} = \sigma \hat{\mathbf{e}}_1$ and $\mathbf{v}_1 = 1$ (see [2, 13]).

Input: $\mathbf{x} \in \mathbb{R}^m$

Output: $\mathbf{v} \in \mathbb{R}^m$, and $\sigma, \beta \in \mathbb{R}$ such that $(I - \beta \mathbf{v} \mathbf{v}^\top) \mathbf{x} = \pm \|\mathbf{x}\|_2 \hat{\mathbf{e}}_1 = \sigma \hat{\mathbf{e}}_1$

253 **1** $\mathbf{v} \leftarrow \text{copy}(\mathbf{x})$
2 $\sigma \leftarrow -\text{sign}(\mathbf{x}_1) \|\mathbf{x}\|_2$
3 $\mathbf{v}_1 \leftarrow \mathbf{x}_1 - \sigma$
4 $\beta \leftarrow -\frac{\mathbf{v}_1}{\sigma}$
5 **return** $\beta, \mathbf{v}/\mathbf{v}_1, \sigma$

Algorithm 3: $\mathbf{V}, \beta, \mathbf{R} = \text{HQR2}(A)$. A Level-2 BLAS implementation of the Householder QR algorithm. Given a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ where $m \geq n$, return matrix $\mathbf{V} \in \mathbb{R}^{m \times n}$, vector $\beta \in \mathbb{R}^n$, and upper triangular matrix \mathbf{R} . An orthogonal matrix \mathbf{Q} can be generated from \mathbf{V} and β , and $\mathbf{Q}\mathbf{R} = \mathbf{A}$.

Input: $A \in \mathbb{R}^{m \times n}$ where $m \geq n$.

Output: $\mathbf{V}, \beta, \mathbf{R}$

1 $\mathbf{V}, \beta \leftarrow \mathbf{0}_{m \times n}, \mathbf{0}_m$
2 **for** $i = 1 : n$ **do**
3 $\mathbf{v}, \beta, \sigma \leftarrow \text{hh_vec}(\mathbf{A}[i : \text{end}, i])$ /* Algorithm 2 */
4 $\mathbf{V}[i : \text{end}, i], \beta_i, \mathbf{A}[i, i] \leftarrow \mathbf{v}, \beta, \sigma$
5 $\mathbf{A}[i + 1 : \text{end}, i] \leftarrow \text{zeros}(m - i)$
6 $\mathbf{A}[i : \text{end}, i + 1 : \text{end}] \leftarrow \mathbf{A}[i : \text{end}, i + 1 : \text{end}] - \beta \mathbf{v} \mathbf{v}^\top \mathbf{A}[i : \text{end}, i + 1 : \text{end}]$
7 **return** $\mathbf{V}, \beta, \mathbf{A}[1 : n, 1 : n]$

254 **3.1.2. HQR: Rounding Error Analysis.** Now we present an error analysis for [alg. 3](#) by
 255 keeping track of the different operations of [alg. 2](#) and [alg. 3](#).

256 *Calculating the i^{th} Householder vector and constant.* In [alg. 3](#), the i^{th} Householder vector
 257 shares all but the first component with the target column, $\mathbf{A}[i : m, i]$. We first calculate σ as is
 258 implemented in line 2 of [alg. 2](#).

$$259 \quad (3.3) \quad \text{fl}(\sigma) = \hat{\sigma} = \text{fl}(-\text{sign}(\mathbf{A}_{i,i}) \|\mathbf{A}[i : m, i]\|_2) = \sigma + \Delta\sigma, \quad |\Delta\sigma| \leq \gamma_{m-i+1} |\sigma|.$$

260 Note that the backward error incurred here is simply that an inner product of a vector in \mathbb{R}^{m-i+1}
 261 with itself. Let $\tilde{\mathbf{v}}_1 \equiv \mathbf{A}_{i,i} - \sigma$, the penultimate value \mathbf{v}_1 . The subtraction adds a single additional

262 rounding error via

$$263 \quad \text{fl}(\tilde{\mathbf{v}}_1) = \tilde{\mathbf{v}}_1 + \Delta\tilde{\mathbf{v}}_1 = (1 + \delta)(\mathbf{A}_{i,i} - \sigma - \Delta\sigma) = (1 + \tilde{\theta}_{m-i+2})(\mathbf{A}_{i,i} - \sigma)$$

264 where the last equality is granted because the sign of σ is chosen to prevent cancellation. For the sake
 265 of simplicity, we write $|\Delta\tilde{\mathbf{v}}_1| \leq \tilde{\gamma}_{m-i+1}|\tilde{\mathbf{v}}_1|$ even though a tighter relative upper bound is θ_{m-i+2}
 266 We sweep that minor difference (in comparison to $\mathcal{O}(m-i)$) under the our use of the $\tilde{\gamma}$ notation
 267 defined in [Lemma 2.1](#). Since [alg. 2](#) normalizes the Householder vector so that its first component
 268 is 1, the remaining components of \mathbf{v} are divided by $\text{fl}(\tilde{\mathbf{v}}_1)$ incurring another single rounding error.
 269 As a result, the rounding errors in \mathbf{v} are

$$270 \quad (3.4) \quad \text{fl}(\mathbf{v}_j) = \mathbf{v}_j + \Delta\mathbf{v}_j \text{ where } |\Delta\mathbf{v}_j| \leq \begin{cases} 0, & j = 1 \\ \tilde{\gamma}_{m-i+1}|\mathbf{v}_j|, & j = 2 : m-i+1. \end{cases}$$

271 Next, we consider the Householder constant, β , as is computed in line 4 of [alg. 2](#).

$$272 \quad (3.5) \quad \hat{\beta} = \text{fl}\left(-\frac{\tilde{\mathbf{v}}_1}{\hat{\sigma}}\right) = -(1 + \delta)\frac{\tilde{\mathbf{v}}_1 + \Delta\tilde{\mathbf{v}}_1}{\sigma + \Delta\sigma}$$

$$273 \quad (3.6) \quad = \frac{(1 + \delta)(1 + \theta_{m-i+1})}{(1 + \theta_{m-i+2})}\beta = (1 + \theta_{3(m-i+2)})\beta$$

$$274 \quad (3.7) \quad = \beta + \Delta\beta, \text{ where } |\Delta\beta| \leq \tilde{\gamma}_{m-i+1}\beta.$$

276 We have shown (3.5) to keep our analysis simple in [section 4](#) and (3.6) and (3.7) show that the error
 277 incurred from calculating of $\|\mathbf{A}[i : m, i]\|_2$ accounts for the vast majority of the rounding error so
 278 far.

279 *Applying a Single Householder Transformation.* Now we consider lines 4-6 of [alg. 3](#). Since
 280 the entries in $\mathbf{A}[i+1 : m, i]$ are simply zeroed out and $\mathbf{A}_{i,i}$ is replaced by σ , we only need to
 281 calculate the errors for applying a Householder transformation with the computed Householder
 282 vector and constant. This is the most crucial building block of the rounding error analysis for any
 283 variant of HQR because the \mathbf{Q} factor is formed by applying the Householder transformations to
 284 the identity and both of the blocked versions in [subsection 3.2](#) and [subsection 3.3](#) require efficient
 285 implementations of this step. In this section, we only consider a level-2 BLAS implementation
 286 of applying the Householder transformation, but in [subsection 3.2](#) we introduce a level-3 BLAS
 287 implementation.

288 A Householder transformation is applied through a series of inner and outer products, since
 289 Householder matrices are rank-1 updates of the identity. That is, computing $\mathbf{P}_{\mathbf{v}}\mathbf{x}$ for any $\mathbf{x} \in \mathbb{R}^m$
 290 is as simple as computing $\mathbf{y} := \mathbf{x} - (\beta\mathbf{v}^\top\mathbf{x})\mathbf{v}$. Let us assume that \mathbf{x} is an exact vector and there
 291 were errors incurred in forming \mathbf{v} and β . The errors incurred from computing \mathbf{v} and β need to be
 292 included in addition to the new rounding errors accumulating from the action of applying $\mathbf{P}_{\mathbf{v}}$ to
 293 a column. In practice, \mathbf{x} would be a column in $\mathbf{A}^{(i-1)}[i+1 : m, i+1 : n]$, where the superscript
 294 $(i-1)$ indicates that this submatrix of \mathbf{A} has already been transformed by $i-1$ Householder
 295 transformations that zeroed out components below $\mathbf{A}_{j,j}$ for $j = 1 : i-1$. We show the error for
 296 forming $\text{fl}(\hat{\mathbf{v}}^\top\mathbf{x})$ where we continue to let $\mathbf{v}, \mathbf{x} \in \mathbb{R}^{m-i+1}$ as would be in the i^{th} iteration of the
 297 for-loop in [alg. 3](#):

$$298 \quad \text{fl}(\hat{\mathbf{v}}^\top\mathbf{x}) = (1 + \theta_{m-i+1})(\mathbf{v} + \Delta\mathbf{v})^\top\mathbf{x}.$$

Set $\mathbf{w} := \beta \mathbf{v}^\top \mathbf{x} \mathbf{v}$. Then,

$$\hat{\mathbf{w}} = (1 + \theta_{m-i+1})(1 + \delta)(1 + \tilde{\delta})(\beta + \Delta\beta)(\mathbf{v} + \Delta\mathbf{v})^\top \mathbf{x}(\mathbf{v} + \Delta\mathbf{v}),$$

where θ_{m-i+1} is from computing the inner product $\hat{\mathbf{v}}^\top \mathbf{x}$, and δ and $\tilde{\delta}$ are from multiplying β , $\text{fl}(\hat{\mathbf{v}}^\top \mathbf{x})$, and $\hat{\mathbf{v}}$ together. Finally, we can add in the vector subtraction operation and complete the rounding error analysis of applying a Householder transformation to any vector:

$$(3.8) \quad \text{fl}(\mathbf{x} - \hat{\mathbf{w}}) = (1 + \delta)(\mathbf{x} - \mathbf{w} - \Delta\mathbf{w}) = (1 + \tilde{\theta}_{m-i+1})\mathbf{y}.$$

We can easily switch between forward and errors from (3.8) via

$$\mathbf{y} + \Delta\mathbf{y} = (1 + \tilde{\theta}_{m-i+1})\mathbf{y} = (1 + \tilde{\theta}_{m-i+1})\mathbf{P}_\mathbf{v}\mathbf{x} = (\mathbf{P}_\mathbf{v} + \Delta\mathbf{P}_\mathbf{v})\mathbf{x},$$

where $|\Delta\mathbf{y}| \leq \tilde{\gamma}_{m-i+1}|\mathbf{y}|$ and $|\Delta\mathbf{P}_\mathbf{v}| \leq \tilde{\gamma}_{m-i+1}|\mathbf{P}_\mathbf{v}|$.

Even though we never explicitly form $\mathbf{P}_\mathbf{v}$, forming the normwise error bound for this matrix makes the analysis for HQR simpler. Therefore, we now transition from componentwise error to matrix norm errors: the 2-norm and the Frobenius norm.

First, we transition from componentwise forward error to the 2-norm forward error via

$$(3.9) \quad \|\Delta\mathbf{y}\|_2 = \left(\sum_{i=1}^m \Delta\mathbf{y}_i^2 \right)^{1/2} \leq \left((\tilde{\gamma}_{m-i+1})^2 \sum_{i=1}^m |\mathbf{y}_i|^2 \right)^{1/2} = \tilde{\gamma}_{m-i+1} \|\mathbf{y}\|_2.$$

In exact arithmetic, we are guaranteed $\|\mathbf{y}\|_2 = \|\mathbf{P}_\mathbf{v}\mathbf{x}\|_2 \leq \|\mathbf{P}\|_2 \|\mathbf{x}\|_2 = \|\mathbf{x}\|_2$ since $\mathbf{P}_\mathbf{v}$ is orthogonal and preserves norms. Combining this with (3.9) we find

$$(3.10) \quad \frac{\|\Delta\mathbf{y}\|_2}{\|\mathbf{x}\|_2} \leq \tilde{\gamma}_{m-i+1}.$$

Now we convert this to a normwise backward error. Since $\Delta\mathbf{P}$ is exactly $\frac{1}{\mathbf{x}^\top \mathbf{x}} \Delta\mathbf{y} \mathbf{x}^\top$, we can compute its Frobenius norm by using $\Delta\mathbf{P}_{ij} = \frac{1}{\|\mathbf{x}\|_2^2} \Delta\mathbf{y}_i \mathbf{x}_j$,

$$(3.11) \quad \|\Delta\mathbf{P}\|_F = \left(\sum_{i=1}^m \sum_{j=1}^m \left(\frac{1}{\|\mathbf{x}\|_2^2} \Delta\mathbf{y}_i \mathbf{x}_j \right)^2 \right)^{1/2} = \frac{\|\Delta\mathbf{y}\|_2}{\|\mathbf{x}\|_2} \leq \tilde{\gamma}_{m-i+1},$$

where the last inequality is a direct application of (3.10). We summarize these results in Lemma 3.2.

LEMMA 3.2. Let $\mathbf{x} \in \mathbb{R}^m$ and consider the computation of $\hat{\mathbf{y}} = \text{fl}(\mathbf{P}_\mathbf{v}\mathbf{x})$ via

$$\mathbf{y} + \Delta\mathbf{y} = \text{fl}(\mathbf{P}_\mathbf{v}\mathbf{x}) = \text{fl}(\mathbf{x} - \hat{\beta} \hat{\mathbf{v}} \hat{\mathbf{v}}^\top \mathbf{x})$$

and rounding errors incurred in forming $\hat{\mathbf{v}}$ and $\hat{\beta}$ are expressed componentwise via $\hat{\mathbf{v}} = \mathbf{v} + \Delta\mathbf{v}$ and $\hat{\beta} = \beta + \Delta\beta$. Let us write the componentwise forward error bound as $|\Delta\mathbf{y}| \leq \gamma_y |\mathbf{y}|$. Then, the normwise forward and backward errors are

$$(3.12) \quad \|\Delta\mathbf{y}\|_2 \leq \gamma_y \|\mathbf{y}\|_2, \quad \|\mathbf{P}_\mathbf{v}\|_F \leq \gamma_y.$$

Note that in a uniform precision setting this bound is represented as $\gamma_y = \tilde{\gamma}_m$, where the majority of the round-off errors are attributed to inner product computations for forming $\hat{\beta}$ and \mathbf{v} .

Applying many successive Householder transformations. Consider applying a sequence of transformations in the set $\{\mathbf{P}_i\}_{i=1}^r \subset \mathbb{R}^{m \times m}$ to $\mathbf{x} \in \mathbb{R}^m$, where \mathbf{P}_i 's are all Householder transformations. This is directly applicable to HQR as $\mathbf{Q} = \mathbf{P}_1 \cdots \mathbf{P}_n \mathbf{I}$ and $\mathbf{R} = \mathbf{Q}^\top \mathbf{A} = \mathbf{P}_n \cdots \mathbf{P}_1 \mathbf{A}$. Let us define

$$\mathbf{Q} + \Delta \mathbf{Q}' \equiv \prod_{i=1}^r (\mathbf{P}_i + \Delta \mathbf{P}_i)$$

in the context of applying this matrix to a vector, $\mathbf{x} \in \mathbb{R}^m$, where $\Delta \mathbf{Q}'^\top$ represents the backward error of forming \mathbf{R} , instead of the forward error of the \mathbf{Q} factor. The forward error for \mathbf{Q} is denoted as $\Delta \mathbf{Q} \equiv \text{fl}(\mathbf{Q}) - \mathbf{Q}$ where $\text{fl}(\mathbf{Q})$ is formed via HQR. That is, if $\mathbf{y} = \mathbf{Q}^\top \mathbf{x}$, then $\text{fl}(\mathbf{y}) = \mathbf{y} + \Delta \mathbf{y} = (\mathbf{Q} + \Delta \mathbf{Q}')^\top \mathbf{x}$. Even though an efficient implementation would use that \mathbf{P}_i 's are applied to successively shorter vectors (\mathbf{P}_i is left multiplied to $\mathbf{A}[i : m, i + 1 : n]$, which is equivalent to $n - i$ vectors of length $m - i + 1$), we assume $\{\mathbf{P}_i\}_{i=1}^r \subset \mathbb{R}^{m \times m}$ to allow for a simpler analysis while forming a looser bound. We will now use Lemma 3.7 from [13] to bound $\Delta \mathbf{Q}'$ with the Frobenius norm.

$$(3.11) \quad \|\Delta \mathbf{Q}'^\top\|_F = \left\| \prod_{i=1}^r (\mathbf{P}_i + \Delta \mathbf{P}_i) - \prod_{i=r}^1 \mathbf{P}_i \right\|_F,$$

$$(3.12) \quad \leq \left(\prod_{i=1}^r (1 + \tilde{\gamma}_m) - 1 \right) \prod_{i=r}^1 \|\mathbf{P}_i\|_2 = (1 + \tilde{\gamma}_m)^r - 1.$$

The last equality results from the orthogonality of Householder matrices, and we further reduce the last term. Generalizing the last rule in Lemma 2.2 yields

$$(1 + \tilde{\gamma}_m)^r = (1 + \tilde{\gamma}_m)^{r-2} (1 + \tilde{\gamma}_m) (1 + \tilde{\gamma}_m) \leq (1 + \tilde{\gamma}_m)^{r-2} (1 + \tilde{\gamma}_{2m}) \leq \cdots \leq (1 + \tilde{\gamma}_{rm}).$$

Now we will use the following equivalent algebraic inequalities to get the final result.

$$(3.13) \quad 0 < a < b < 1 \Leftrightarrow 1 - a > 1 - b \Leftrightarrow \frac{1}{1 - a} < \frac{1}{1 - b} \Leftrightarrow \frac{a}{1 - a} < \frac{b}{1 - b}$$

In addition, we assume $r\tilde{\gamma}_m < \frac{1}{2}$, such that

$$(3.14) \quad (1 + \tilde{\gamma}_m)^r - 1 \leq \gamma_w^{(r\tilde{z})} = \frac{r\tilde{z}u_w}{1 - r\tilde{z}u_w} \quad (\text{by definition})$$

$$(3.15) \quad \leq \frac{r\tilde{\gamma}_m}{1 - r\tilde{\gamma}_m}, \text{ since } r\tilde{z}u_w < r\tilde{\gamma}_m \quad (\text{by Equation 3.13})$$

$$(3.16) \quad \leq 2r\tilde{\gamma}_m \quad (\text{since } r\tilde{\gamma}_m < \frac{1}{2} \text{ implies } \frac{1}{1 - r\tilde{\gamma}_m} < 2)$$

$$(3.17) \quad = r\tilde{\gamma}_m,$$

Therefore, we have $(1 + \tilde{\gamma}_m)^r - 1 \leq r\tilde{\gamma}_m$ and

$$(3.18) \quad \|\Delta \mathbf{Q}'\|_2 \leq \|\Delta \mathbf{Q}'\|_F = \|\Delta \mathbf{Q}'^\top\|_F \leq r\tilde{\gamma}_m$$

In this current uniform precision error analysis, the important quantity $\tilde{\gamma}_m$ is derived from the backward error of applying one Householder transformation. To easily generalize this section for

mixed-precision analysis, we benefit from alternatively denoting this quantity as $\tilde{\gamma}_{\mathbf{P}}$ with the understanding that $\tilde{\gamma}_{\mathbf{P}}$ will be some combination of $\tilde{\gamma}$'s of differing precisions. Equation (3.17) would then be

$$(3.19) \quad (1 + \tilde{\gamma}_{\mathbf{P}})^r - 1 \leq r\tilde{\gamma}_{\mathbf{P}}.$$

Next, we apply (3.18) to the i^{th} columns of \mathbf{Q}, \mathbf{R} and set $r = n$ for a full rank matrix, \mathbf{A} . Then,

$$\begin{aligned} \|\Delta \mathbf{R}[:, i]\|_2 &= \|\Delta \mathbf{Q}'^\top \mathbf{A}[:, i]\|_2 \leq \|\Delta \mathbf{Q}'\|_2 \|\mathbf{A}[:, i]\|_2 \leq n\tilde{\gamma}_m \|\mathbf{A}[:, i]\|_2, \\ \|\Delta \mathbf{Q}[:, i]\|_2 &= \|\Delta \mathbf{Q}' \mathbf{I}[:, i]\|_2 \leq \|\Delta \mathbf{Q}'\|_2 \leq n\tilde{\gamma}_m. \end{aligned}$$

These columnwise bounds can now be transformed into matrix norms as follows:

$$\begin{aligned} \|\Delta \mathbf{R}\|_F &= \left(\sum_{i=1}^n \|\Delta \mathbf{R}[:, i]\|_2^2 \right)^{1/2} \leq \left(\sum_{i=1}^n n^2 \tilde{\gamma}_m^2 \|\mathbf{A}[:, i]\|_2^2 \right)^{1/2} = n\tilde{\gamma}_m \|\mathbf{A}\|_F, \\ \|\Delta \mathbf{Q}\|_F &= \left(\sum_{i=1}^n \|\Delta \mathbf{Q}[:, i]\|_2^2 \right)^{1/2} \leq \left(\sum_{i=1}^n \tilde{\gamma}_m^2 \right)^{1/2} = n^{3/2} \tilde{\gamma}_m. \end{aligned}$$

We gather these results into Theorem 3.3.

THEOREM 3.3. *Let $\mathbf{A} \in \mathbb{R}^{m \times n}$ with $m \geq n$ have full rank, n . Let $\hat{\mathbf{Q}} \in \mathbb{R}^{m \times n}$ and $\hat{\mathbf{R}} \in \mathbb{R}^{n \times n}$ be the thin QR factors of \mathbf{A} obtained via alg. 3, defined via*

$$\begin{aligned} \hat{\mathbf{R}} &= \mathbf{R} + \Delta \mathbf{R} = \text{fl}(\hat{\mathbf{P}}_n \cdots \hat{\mathbf{P}}_1 \mathbf{A}), \quad n\tilde{\gamma}_m \|\mathbf{A}\|_F \\ \hat{\mathbf{Q}} &= \mathbf{Q} + \Delta \mathbf{Q} = \text{fl}(\hat{\mathbf{P}}_1 \cdots \hat{\mathbf{P}}_n \mathbf{I}), \quad \|\Delta \mathbf{Q}\|_F \leq n^{3/2} \tilde{\gamma}_m. \end{aligned}$$

Let $\mathbf{A} + \Delta \mathbf{A} = \hat{\mathbf{Q}} \hat{\mathbf{R}}$, where $\hat{\mathbf{Q}}$ and $\hat{\mathbf{R}}$ are obtained via Algorithm 3. Then the backward error is

$$(3.20) \quad \|\Delta \mathbf{A}\|_F \leq n^{3/2} \tilde{\gamma}_m \|\mathbf{A}\|_F.$$

The content of this section is largely derived directly from [13], but we kept the analysis general by employing quantities denoted via $\Delta\beta$, $\Delta\mathbf{v}$, $\tilde{\gamma}_y$, and $\tilde{\gamma}_{\mathbf{P}}$. These quantities account for various forward and backward errors formed in computing essential components of HQR, namely the Householder constant and vector, as well as normwise errors of the action of applying Householder transformations. In the next sections, we present blocked variants of HQR that use alg. 3.

3.2. Block HQR with partitioned columns (BQR). We refer to the blocked variant of HQR where the columns are partitioned as BQR. Note that this algorithm relies on the WY representation described in [4] instead of the storage-efficient version of [19].

3.2.1. The WY Representation. A convenient matrix representation that accumulates r Householder reflectors is known as the WY representation (see [4, 10]). Lemma 3.4 shows how to update a rank- j update of the identity, $\mathbf{Q}^{(j)}$, with a Householder transformation, \mathbf{P} , to produce a rank- $(j+1)$ update of the identity, $\mathbf{Q}^{(j+1)}$. With the correct initialization of \mathbf{W} and \mathbf{Y} , we can build the WY representation of successive Householder transformations as shown in Algorithm 4.

LEMMA 3.4. *Suppose $\mathbf{Q}^{(j)} = \mathbf{I} - \mathbf{W}^{(j)} \mathbf{Y}^{(j)\top} \in \mathbb{R}^{m \times m}$ is an orthogonal matrix with $\mathbf{W}^{(j)}, \mathbf{Y}^{(j)} \in \mathbb{R}^{m \times j}$. Let us define $\mathbf{P} = \mathbf{I} - \beta \mathbf{v} \mathbf{v}^\top$ for some $\mathbf{v} \in \mathbb{R}^m$ and let $\mathbf{z}^{(j+1)} = \beta \mathbf{Q}^{(j)} \mathbf{v}$. Then,*

$$\mathbf{Q}^{(j+1)} = \mathbf{Q}^{(j)} \mathbf{P} = \mathbf{I} - \mathbf{W}^{(j+1)} \mathbf{Y}^{(j+1)\top},$$

where $\mathbf{W}^{(j+1)} = [\mathbf{W}^{(j)} | \mathbf{z}]$ and $\mathbf{Y}^{(j+1)} = [\mathbf{Y}^{(j)} | \mathbf{v}]$ are each m -by- $(j+1)$.

Algorithm 4: $\mathbf{W}, \mathbf{Y} \leftarrow \text{buildWY}(V, \beta)$: Given a set of householder vectors $\{\mathbf{V}[:, i]\}_{i=1}^r$ and their corresponding constants $\{\beta_i\}_{i=1}^r$, form the final \mathbf{W} and \mathbf{Y} factors of the WY representation of $\mathbf{P}_1 \cdots \mathbf{P}_r$, where $\mathbf{P}_i := \mathbf{I}_m - \beta_i \mathbf{v}_i \mathbf{v}_i^\top$

Input: $\mathbf{V} \in \mathbb{R}^{m \times r}$, $\beta \in \mathbb{R}^r$ where $m > r$.

Output: \mathbf{W}, \mathbf{Y}

```

1 Initialize:  $\mathbf{W} := \beta_1 \mathbf{V}[:, 1]$  and  $\mathbf{Y} := \mathbf{V}[:, 1]$ .
2 for  $j = 2 : r$  do
3    $\mathbf{z} \leftarrow \beta_j [\mathbf{V}[:, j] - \mathbf{W} (\mathbf{Y}^\top \mathbf{V}[:, j])]$ 
4    $\mathbf{W} \leftarrow [\mathbf{W} \quad \mathbf{z}]$  /* Update  $\mathbf{W}$ . */
5    $\mathbf{Y} \leftarrow [\mathbf{Y} \quad \mathbf{V}[:, j]]$  /* Update  $\mathbf{Y}$ . */
   //  $\mathbf{W}$  and  $\mathbf{Y}$  are now  $m$ -by- $j$  matrices.
6 return  $\mathbf{W}, \mathbf{Y}$ 
```

In HQR, \mathbf{A} is transformed into an upper triangular matrix \mathbf{R} by identifying a Householder transformation that zeros out a column below the diagonal, then applying that Householder transformation to the bottom right partition. For example, the k^{th} Householder transformation finds an $m - k + 1$ sized Householder transformation that zeros out column k below the diagonal and then applies it to the $(m - k + 1)$ -by- $(n - k)$ partition of the matrix, $\mathbf{A}[k : m, k + 1 : n]$. Since the $k + 1^{\text{st}}$ column is transformed by the k^{th} Householder transformation, this algorithm must be executed serially as shown in [alg. 3](#). The highest computational burden at each iteration falls on [alg. 3](#) line 6, which requires Level-2 BLAS operations when computed efficiently.

In contrast, BQR replaces this step with Level-3 BLAS operations by partitioning \mathbf{A} by groups of columns. Let $\mathbf{A} = [\mathbf{C}_1 \cdots \mathbf{C}_N]$ where $\mathbf{C}_1, \dots, \mathbf{C}_{N-1}$ are each m -by- r , and \mathbf{C}_N holds the remaining columns. The k^{th} block, \mathbf{C}_k , is transformed using HQR ([alg. 3](#)) while building the WY representation of $\mathbf{P}_{(k-1)r+1} \cdots \mathbf{P}_{kr} = \mathbf{I}_m - \mathbf{W}_k \mathbf{Y}_k^\top$ as in [alg. 4](#). Note that both [algs. 3](#) and [4](#) are rich in Level-2 BLAS operations. Then, $\mathbf{I} - \mathbf{Y}_k \mathbf{W}_k^\top$ is applied to $[\mathbf{C}_2 \cdots \mathbf{C}_N]$ with two Level-3 BLAS operations as shown in line 6 of [alg. 5](#). BQR performs approximately $1 - \mathcal{O}(1/N)$ fraction of its FLOPs in Level-3 BLAS operations (see section 5.2.3 of [10]), and can reap the benefits from the accelerated matrix-matrix-multiply and accumulate technology of TensorCore. Note that BQR does require more FLOPs when compared to HQR, but these additional FLOPs are negligible in high precision. A pseudoalgorithm for BQR is shown in [alg. 5](#).

3.2.2. BQR: Rounding Error Analysis. We now present the basic structure for the rounding error analysis for [alg. 5](#), which consist of: 1)HQR, 2)building the WY representation, and 3) updating the remaining blocks with the WY representation.

HQR within each block. Consider the k^{th} block, \mathbf{C}_k . We first apply [Algorithm 3](#) to rows $k : m$, which is equivalent to r Householder transformations of size $m - (r - 1)k$ if $k < N$ and $n - r(i - 1)$ Householder transformations of size $m - (N - 1)k$ if $k = N$. The general rounding error incurred is represented by (3.11) and a uniform-precision rounding error for this step is shown in (3.12). Let \mathbf{R}_k be the \mathbf{R} factor acquired from applying HQR on \mathbf{C}_k and let $\Delta \mathbf{Q}'_k$ represent the backward error incurred in this step:

$$\mathbf{R}_k = (\mathbf{Q}_k + \Delta \mathbf{Q}'_k)^\top \mathbf{C}_k.$$

Algorithm 5: $\mathbf{Q}, \mathbf{R} \leftarrow \text{blockHQR}(\mathbf{A}, r)$: Perform Householder QR factorization of matrix \mathbf{A} with column partitions of size r .

Input: $\mathbf{A} \in \mathbb{R}^{m \times n}$, $r \in \mathbb{R}$ where $r < n$.
Output: \mathbf{Q}, \mathbf{R}

```

1  $N = \lceil \frac{n}{r} \rceil$ 
  // Let  $\mathbf{A} = [\mathbf{C}_1 \cdots \mathbf{C}_N]$  where all blocks except  $\mathbf{C}_N$  are  $m$ -by- $r$  sized.
2 for  $i = 1 : N$  do
3    $\mathbf{V}_i, \beta_i, \mathbf{C}_i \leftarrow \text{hhQR}(\mathbf{C}_i)$                                      /* Algorithm 3 */
4    $\mathbf{W}_i, \mathbf{Y}_i \leftarrow \text{buildWY}(\mathbf{V}_i, \beta_i)$                              /* Algorithm 4 */
5   if  $i < N$  then
6      $\lfloor [\mathbf{C}_{i+1} \cdots \mathbf{C}_N] := \mathbf{Y}_i (\mathbf{W}_i^\top [\mathbf{C}_{i+1} \cdots \mathbf{C}_N])$       /* update the rest: BLAS-3 */
  //  $\mathbf{A}$  has been transformed into  $\mathbf{R} = \mathbf{Q}^\top \mathbf{A}$ .
  // Now build  $\mathbf{Q}$  using level-3 BLAS operations.
7  $\mathbf{Q} \leftarrow \mathbf{I}$                                                          /*  $\mathbf{I}_m$  if full QR, and  $\mathbf{I}_{m \times n}$  if thin QR. */
8 for  $i = N : -1 : 1$  do
9    $\lfloor \mathbf{Q}[(i-1)r+1 : m, (i-1)r+1 : n] = \mathbf{W}_i (\mathbf{Y}_i^\top \mathbf{Q}[(i-1)r+1 : m, (i-1)r+1 : n])$ 
10 return  $\mathbf{Q}, \mathbf{A}$ 
```

419 Adjusting (3.11) and (3.12) for $k < N$ yields

$$420 \quad (3.21) \quad \|\Delta \mathbf{Q}'_k\|_F = \left\| \prod_{j=r}^1 (\mathbf{P}_{(k-1)r+j} + \Delta \mathbf{P}_{(k-1)r+j}) - \prod_{j=r}^1 \mathbf{P}_{(k-1)r+j} \right\|_F,$$

$$421 \quad (3.22) \quad \leq \left(\prod_{i=1}^r (1 + \tilde{\gamma}_{m-(r-1)k}) - 1 \right) \prod_{i=r}^1 \|\mathbf{P}_i\|_2 = (1 + \tilde{\gamma}_{m-(r-1)k})^r - 1.$$

422

423 *Build WY at each block.* We now calculate the rounding errors incurred from building the WY
424 representation when given a set of Householder vectors and constants. Consider the j^{th} update as
425 shown in Lemma 3.4 for the k^{th} block. Error accumulated from forming \mathbf{v} is represented in (3.4)
426 and we only consider $\mathbf{z}^{(j+1)} = \beta \mathbf{Q}^{(j)} \mathbf{v}$. Since $\mathbf{Q}^j = \mathbf{I} - \mathbf{W}^{(j)} \mathbf{Y}^{(j)\top}$, let's first consider $\mathbf{W}^{(j)} \mathbf{Y}^{(j)\top} \mathbf{v}$
427 where we left-multiply the matrices. In general, we can write

$$428 \quad \mathbf{z}^{(j+1)} + \Delta \mathbf{z}^{(j+1)} = \hat{\mathbf{v}} - (\mathbf{W}^{(j)} + \Delta \mathbf{W}^{(j)}) (\mathbf{Y}^{(j)} + \Delta \mathbf{Y}^{(j)})^\top \hat{\mathbf{v}},$$

429 where $\hat{\mathbf{v}}$ is expressed in (3.4), and $\Delta \mathbf{W}^{(j)}$ and $\Delta \mathbf{Y}^{(j)}$ each represent backward rounding errors from
430 $m - (r-1)k$ -length and j -length dot products. In uniform precision, this yields

$$431 \quad \text{fl}(\mathbf{W}^{(j)} \mathbf{Y}^{(j)\top} \mathbf{v}) = (1 + \tilde{\theta}_{m-(k-1)r}) (1 + \tilde{\theta}_j) \mathbf{W}^{(j)} \mathbf{Y}^{(j)\top} \mathbf{v} = (1 + \tilde{\theta}_{j+m-(k-1)r}) \mathbf{W}^{(j)} \mathbf{Y}^{(j)\top} \mathbf{v},$$

432 where we've disregarded $\Delta \mathbf{v}$ momentarily. The subtraction and the multiplication by β only add
433 in δ each to the errors, so we simplify via $j + m - (k-1)r + 2 \approx m - rk$ since $j \leq r$. Since
434 $|\Delta \mathbf{v}| \leq \tilde{\gamma}_{m-(k-1)r} |\mathbf{v}|$, the approximation still holds. Thus, we result in

$$435 \quad \text{fl}(\mathbf{z}^{(j+1)}) = (1 + \tilde{\theta}_{m-rk}) \mathbf{z}^{(j+1)}.$$

3.3. Block HQR with partitioned rows : Tall-and-Skinny QR (TSQR).

4. Mixed-precision error analysis.

4.1. Round down at the end of the factorization.

4.2. Round down at block-level (BLAS-3).

4.3. Round down at inner-product level (BLAS-2).

5. Numerical Experiments.

6. Conclusion. Though the use of lower precision naturally reduces the bandwidth and storage needs, the development of GPUs to optimize low precision floating point arithmetic have accelerated the interest in half precision and mixed-precision algorithms. Loss in precision, stability, and representable range offset for those advantages, but these shortcomings may have little to no impact in some applications. It may even be possible to navigate around those drawbacks with algorithmic design.

The existing rounding error analysis cannot accurately bound the behavior of mixed-precision arithmetic. We have developed a new framework for mixed-precision rounding error analysis and applied it to HQR, a widely used linear algebra routine, and implemented it in an iterative eigensolver in the context of spectral clustering. The mixed-precision error analysis builds from the inner product routine, which can be applied to many other linear algebra tools as well. The new error bounds more accurately describe how rounding errors are accumulated in mixed-precision settings. We also found that TSQR, a communication-avoiding, easily parallelizable QR factorization algorithm for tall-and-skinny matrices, can outperform HQR in mixed-precision settings for ill-conditioned, extremely overdetermined cases, which suggests that some algorithms are more robust against lower precision arithmetic. As QR factorizations of tall-and-skinny matrices are common in spectral clustering, we experimented with introducing mixed-precision settings into graph partitioning problems. In particular, we applied DBSCAN to the spectral basis of a graph identified via subspace iteration that used our simulated mixed-precision HQR, which yielded clustering results tantamount to results from employing double-precision entirely.

Although this work is focused on QR factorizations and applications in spectral clustering, the mixed precision round-off error analysis can be applied to other tasks and applications that can benefit from employing low precision computations. While the emergence of technology that support low precision floats combats issues dealing with storage, now we need to consider how low precision affects stability of numerical algorithms.

Future work is needed to test larger, more ill-conditioned problems with different mixed-precision settings, and to explore other divide-and-conquer methods like TSQR that can harness parallel capabilities of GPUs while withstanding lower precisions.

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