

# 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 [12] 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 [?] or training dense neural networks [17], 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 [?]. 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 [10, 11], (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 [2]. 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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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 and was supported by the LLNL-LDRD Program under Project No. 17-SI-004, LLNL-JRNL-795525-DRAFT.

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
$b, t, \mu, \eta$	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
$\delta^{(q)}$	Quantity bounded by: $ \delta^{(q)}  < u^{(q)}$	2.1
$\gamma_k^{(q)}, \theta_k^{(q)}$	$\frac{ku^{(q)}}{1-ku^{(q)}}$ , 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  $\mu$  is any integer in  $[0, b^t - 1]$  and  $\eta$  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 [12], which allow a relatively simple framework for formulating error bounds for complex linear algebra operations. A short analysis of FLOPs (see Theorem 2.2 [12]) 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	$\eta_{\min}$	$\eta_{\max}$	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,  $\delta$ , 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 [12]). 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  $\theta$  so that  $|\tilde{\theta}_k| \leq \tilde{\gamma}_k$ .

103 In other words,  $\theta_k$  represents the accumulation of rounding errors from  $k$  successive operations, and  
 104 it is bounded by  $\gamma_k$ . Allowing  $\theta_k$ 's to be any arbitrary value within the corresponding  $\gamma_k$  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 [12]. 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  $\gamma_m$ , 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 [14], 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 [13, 16]) 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.

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**Algorithm 1:**  $\mathbf{z}^{(\text{fp16})} = \text{simHalf}(f, \mathbf{x}^{(\text{fp16})}, \mathbf{y}^{(\text{fp16})})$ . Simulate function  $f \in \text{OPU}\{\text{dot\_product}\}$  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.

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**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  $\mathbf{z}^{(\text{fp16})}$ 
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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 [12] that build on Lemma 2.1 in Lemma 2.2. These rules summarize how to accumulate errors represented by  $\theta$ 's and  $\gamma$ '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. In Lemma 2.3, we present just a few rules adapted for multiple precisions from Lemma 2.2 that we will use repeatedly in future sections.

LEMMA 2.2. For any positive integer  $k$ , let  $\theta_k$  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  $\theta_k$ '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  $\gamma$ '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 integers  $k_l, k_h$  and some precision  $q$  defined with respect to the unit round-off,  $u^{(q)}$ , define  $\gamma_k^{(q)} := \frac{ku^{(q)}}{1-ku^{(q)}}$ . Consider a low precision and a high precision where  $1 \gg u_l \gg u_h > 0$ . Then,

$$\begin{aligned} \gamma_{k_h}^{(h)} \gamma_{k_l}^{(l)} &\leq \gamma_{k_l}^{(l)}, \quad \text{for } k_h u^{(h)} \leq \frac{1}{2}, \\ \gamma_{k_h}^{(h)} + u^{(l)} &\leq \gamma_{d_1}^{(l)}, \\ \gamma_{k_l}^{(l)} + u^{(h)} &\leq \gamma_{k_l+1}^{(l)}, \\ \gamma_{k_l}^{(l)} + \gamma_{k_h}^{(h)} + \gamma_{k_l}^{(l)} \gamma_{k_h}^{(h)} &< \gamma_{k_l+d_2}^{(l)}, \end{aligned}$$

where  $d_1 = \lceil (u^{(l)} + k_h u^{(h)}) / u^{(l)} \rceil$  and  $d_2 = \lceil k_h u^{(h)} / u^{(l)} \rceil$ .

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 a 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. 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 precisions and exponent ranges. 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  $\eta_x, \eta_y \in [-15, 16]$ , and note that the significand and exponent range for fp32 are  $[0, 2^{24} - 1]$  and  $[-127, 128]$ . Then the product in full precision 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  $\eta_x + \eta_y + 2 \in [-28, 34] \subseteq [-127, 128]$ , and therefore is exact. Thus, the summation and the final cast down operations are the only sources of rounding error.

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  $l$ .*

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

$$\hat{s}_1 = \text{fl}(\mathbf{x}[1]\mathbf{y}_1) = \mathbf{x}[1]\mathbf{y}_1,$$

$$\hat{s}_2 = \text{fl}(\hat{s}_1 + \mathbf{x}_2\mathbf{y}_2) = (\mathbf{x}[1]\mathbf{y}_1 + \mathbf{x}_2\mathbf{y}_2)(1 + \delta_1^{(h)}),$$

$$\hat{s}_3 = \text{fl}(\hat{s}_2 + \mathbf{x}_3\mathbf{y}_3) = \left[ (\mathbf{x}[1]\mathbf{y}_1 + \mathbf{x}_2\mathbf{y}_2)(1 + \delta_1^{(h)}) + \mathbf{x}_3\mathbf{y}_3 \right] (1 + \delta_2^{(h)}).$$

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

$$(2.9) \quad \hat{s}_m = (\mathbf{x}[1]\mathbf{y}_1 + \mathbf{x}_2\mathbf{y}_2) \prod_{k=1}^{m-1} (1 + \delta_k^{(h)}) + \sum_{i=3}^n \mathbf{x}_i\mathbf{y}_i \left( \prod_{k=i-1}^{m-1} (1 + \delta_k^{(h)}) \right).$$

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

$$(2.10) \quad \text{fl}(\mathbf{x}^\top \mathbf{y}) = (\mathbf{x} + \Delta \mathbf{x})^\top \mathbf{y} = \mathbf{x}^\top (\mathbf{y} + \Delta \mathbf{y}), \quad \text{for } |\Delta \mathbf{x}| \leq \gamma_{m-1}^{(h)} |\mathbf{x}|, \quad |\Delta \mathbf{y}| \leq \gamma_{m-1}^{(h)} |\mathbf{y}|.$$

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

$$(2.11) \quad \text{fl}(\mathbf{x}^\top \mathbf{y}) = (\mathbf{x} + \Delta \mathbf{x})^\top \mathbf{y} = \mathbf{x}^\top (\mathbf{y} + \Delta \mathbf{y}), \quad \text{for } |\Delta \mathbf{x}| \leq \gamma_d^{(l)} |\mathbf{x}|, \quad |\Delta \mathbf{y}| \leq \gamma_d^{(l)} |\mathbf{y}|.$$

Equations (2.10) and (2.11) 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  $\mathbf{C} = \mathbf{AB} \in \mathbb{F}_{\text{fp16}}^{p \times q}$ . If  $\text{fl}(\mathbf{C})$  is desired in fp16, then each component of that matrix incurs rounding errors as shown in (2.11) and if it is desired in fp32, the componentwise rounding error is given by (2.10). 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 (2.10) can be used before the cast down operations, and the action of the cast down is best represented by error bounds similar to (2.11).

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.

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

220 **3.1. Householder QR (HQR).** The HQR algorithm uses Householder transformations to  
 221 zero out elements below the diagonal of a matrix (see [15]). We present this as zeroing out all but  
 222 the first element of some vector,  $\mathbf{x} \in \mathbb{R}^m$ .

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

$$225 \quad (3.1) \quad \begin{aligned} \sigma &= -\text{sign}(\mathbf{x}[1])\|\mathbf{x}\|_2, \quad \mathbf{v} = \mathbf{x} - \sigma\hat{\mathbf{e}}_1, \\ \beta &= \frac{2}{\mathbf{v}^\top \mathbf{v}} = -\frac{1}{\sigma \mathbf{v}[1]}, \quad \mathbf{P}_\mathbf{v} = \mathbf{I}_m - \beta \mathbf{v} \mathbf{v}^\top. \end{aligned}$$

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

228 **3.1.1. HQR: Algorithm.** Given  $\mathbf{A} \in \mathbb{R}^{m \times n}$  and Lemma 3.1, HQR is done by repeating the  
 229 following processes until only an upper triangle matrix remains. For  $i = 1, 2, \dots, n$ ,  
 230 Step 1) Compute  $\mathbf{v}$  and  $\beta$  that zeros out the  $i^{\text{th}}$  column of  $\mathbf{A}$  beneath  $a_{ii}$  (see alg. 2), and  
 231 Step 2) Apply  $\mathbf{P}_\mathbf{v}$  to the bottom right partition,  $\mathbf{A}[i : m, i : n]$  (lines 4-6 of alg. 3).

232 Consider the following 4-by-3 matrix example adapted from [12]. Let  $\mathbf{P}_i$  represent the  $i^{\text{th}}$   
 233 Householder transformation of this algorithm.

$$234 \quad \mathbf{A} = \begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix} \xrightarrow{\text{apply } \mathbf{P}_1 \text{ to } \mathbf{A}} \left[ \begin{array}{c|cc} \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{array} \right] \xrightarrow{\text{apply } \mathbf{P}_2 \text{ to } \mathbf{P}_1 \mathbf{A}}$$

$$235$$

$$236 \quad \left[ \begin{array}{cc|c} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{array} \right] \xrightarrow{\text{apply } \mathbf{P}_3 \text{ to } \mathbf{P}_2 \mathbf{P}_1 \mathbf{A}} \left[ \begin{array}{ccc} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & 0 \end{array} \right] = \mathbf{P}_3 \mathbf{P}_2 \mathbf{P}_1 \mathbf{A} =: \mathbf{R}$$

237 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  
 238 thin factors for a general matrix  $\mathbf{A} \in \mathbb{R}^{m \times n}$  are

$$239 \quad (3.2) \quad \mathbf{Q}_{\text{thin}} = \mathbf{P}_1 \cdots \mathbf{P}_n \mathbf{I}_{m \times n} \quad \text{and} \quad \mathbf{R}_{\text{thin}} = \mathbf{I}_{m \times n}^\top \mathbf{P}_n \cdots \mathbf{P}_1 \mathbf{A}.$$



---

**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 [?, 12]).

---

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

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

---

```

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  $\beta$ , and  $\mathbf{QR} = \mathbf{A}$ .

---

**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  $\mathbf{V}, \beta, \mathbf{A}[1 : n, 1 : n]$ 

```

---

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

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

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

Note that the backward error incurred here is simply that an inner product of a vector in  $\mathbb{R}^{m-i+1}$  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 rounding error via

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

where the last equality is granted because the sign of  $\sigma$  is chosen to prevent cancellation. For the sake 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  $\theta_{m-i+2}$ . We sweep that minor difference (in comparison to  $\mathcal{O}(m-i)$ ) under the our use of the  $\tilde{\gamma}$  notation defined in [Lemma 2.1](#). Since [alg. 2](#) normalizes the Householder vector so that its first component is 1, the remaining components of  $\mathbf{v}$  are divided by  $\text{fl}(\tilde{\mathbf{v}}_1)$  incurring another single rounding error.

256 As a result, the rounding errors in  $\mathbf{v}$  are

$$257 \quad (3.4) \quad \text{fl}(\mathbf{v}_j) = \mathbf{v}_j + \Delta \mathbf{v}_j \text{ where } |\Delta \mathbf{v}_j| \leq \begin{cases} 0, & j = 1 \\ \tilde{\gamma}_{m-i+1} |\mathbf{v}_j|, & j = 2 : m - i + 1. \end{cases}$$

258 Next, we consider the Householder constant,  $\beta$ , as is computed in line 4 of [alg. 2](#).

$$259 \quad (3.5) \quad \hat{\beta} = \text{fl} \left( -\frac{\mathbf{v}[1]}{\hat{\sigma}} \right) = -(1 + \delta) \frac{\tilde{\mathbf{v}}_1 + \Delta \tilde{\mathbf{v}}_1}{\sigma + \Delta \sigma}$$

$$260 \quad (3.6) \quad = \frac{(1 + \delta)(1 + \theta_{m-i+1})}{(1 + \theta_{m-i+2})} \beta = (1 + \theta_{3(m-i+2)}) \beta$$

$$261 \quad (3.7) \quad = \beta + \Delta \beta, \text{ where } |\Delta \beta| \leq \tilde{\gamma}_{m-i+1} \beta.$$

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

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

275 A Householder transformation is applied through a series of inner and outer products, since  
276 Householder matrices are rank-1 updates of the identity. That is, computing  $\mathbf{P}_{\mathbf{v}} \mathbf{x}$  for any  $\mathbf{x} \in \mathbb{R}^m$   
277 is as simple as computing

$$278 \quad (3.8) \quad \mathbf{y} := \mathbf{x} - (\beta \mathbf{v}^\top \mathbf{x}) \mathbf{v}.$$

279 Let us assume that  $\mathbf{x}$  is an exact vector and there were errors incurred in forming  $\mathbf{v}$  and  $\beta$ . The  
280 errors incurred from computing  $\mathbf{v}$  and  $\beta$  need to be included in addition to the new rounding errors  
281 accumulating from the action of applying  $\mathbf{P}_{\mathbf{v}}$  to a column. In practice,  $\mathbf{x}$  would be a column in  
282  $\mathbf{A}^{(i-1)}[i + 1 : m, i + 1 : n]$ , where the superscript  $(i - 1)$  indicates that this submatrix of  $\mathbf{A}$  has  
283 already been transformed by  $i - 1$  Householder transformations that zeroed out components below  
284  $\mathbf{A}_{j,j}$  for  $j = 1 : i - 1$ . We show the error for forming  $\text{fl}(\hat{\mathbf{v}}^\top \mathbf{x})$  where we continue to let  $\mathbf{v}, \mathbf{x} \in \mathbb{R}^{m-i+1}$   
285 as would be in the  $i^{\text{th}}$  iteration of the for-loop in [alg. 3](#):

$$286 \quad \text{fl}(\hat{\mathbf{v}}^\top \mathbf{x}) = (1 + \theta_{m-i+1})(\mathbf{v} + \Delta \mathbf{v})^\top \mathbf{x}.$$

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

$$288 \quad \hat{\mathbf{w}} = (1 + \theta_{m-i+1})(1 + \delta)(1 + \tilde{\delta})(\beta + \Delta \beta)(\mathbf{v} + \Delta \mathbf{v})^\top \mathbf{x}(\mathbf{v} + \Delta \mathbf{v}),$$

289 where  $\theta_{m-i+1}$  is from computing the inner product  $\hat{\mathbf{v}}^\top \mathbf{x}$ , and  $\delta$  and  $\tilde{\delta}$  are from multiplying  $\beta$ ,  
290  $\text{fl}(\hat{\mathbf{v}}^\top \mathbf{x})$ , 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:

$$(3.9) \quad \text{fl}(\hat{\mathbf{P}}_{\mathbf{v}}\mathbf{x}) = \text{fl}(\mathbf{x} - \hat{\mathbf{w}}) = (1 + \delta)(\mathbf{x} - \mathbf{w} - \Delta\mathbf{w}) = \mathbf{y} + \Delta\mathbf{y},$$

where  $|\Delta\mathbf{y}| \leq u|\mathbf{x}| + \tilde{\gamma}_{m-i+1}|\beta||\mathbf{v}||\mathbf{v}|^\top|\mathbf{x}|$ . Using  $\sqrt{2/\beta} = \|\mathbf{v}\|_2$ , we can conclude

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

Next, we convert this to a backward error for  $\mathbf{P}_{\mathbf{v}}$ . Since  $\Delta\mathbf{P}_{\mathbf{v}}$  is exactly  $\frac{1}{\mathbf{x}^\top\mathbf{x}}\Delta\mathbf{y}\mathbf{x}^\top$ , we can compute its Frobenius norm by using  $\Delta\mathbf{P}[i, j] = \frac{1}{\|\mathbf{x}\|_2^2}\Delta\mathbf{y}[i]\mathbf{x}[j]$ ,

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

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

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

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  $\hat{\beta} = \beta + \Delta\beta$  where the relative componentwise errors for both are bounded by quantity  $\gamma_y$ :

$$(3.12) \quad |\Delta\mathbf{v}| \leq \gamma_y|\mathbf{v}|, \quad |\Delta\beta| \leq \gamma_y|\beta|.$$

Then, the normwise forward and backward errors are  $\|\Delta\mathbf{y}\|_2 \leq \gamma_y\|\mathbf{y}\|_2$  and  $\|\Delta\mathbf{P}_{\mathbf{v}}\|_F \leq \gamma_y$ .

Note that in a uniform precision setting this bound is represented as  $\gamma_y = \tilde{\gamma}_m$ .

Applying many successive Householder transformations. Consider applying a sequence of transformations in the set  $\{bbP_i\}_{i=1}^r \subset \mathbb{R}^{m \times m}$  to  $\mathbf{x} \in \mathbb{R}^m$ , where  $\mathbf{P}_i$ 's are all Householder transformations computed with  $\tilde{\mathbf{v}}_i$ 's and  $\hat{\beta}_i$ 's. This is directly applicable to HQR as  $\mathbf{Q} = \mathbf{P}_1 \cdots \mathbf{P}_n \mathbf{I}$  and  $\mathbf{R} = \mathbf{Q}^\top \mathbf{A} = \mathbf{P}_n \cdots \mathbf{P}_1 \mathbf{A}$ . [Lemma 3.3](#) is very useful for any sequence of transformations, where each transformation has a known bound. We will invoke this lemma to prove [Lemma 3.4](#), and use it in future sections for other sequential transformations.

LEMMA 3.3. If  $\mathbf{X}_j + \Delta\mathbf{X}_j \in \mathbb{R}^{m \times m}$  satisfies  $\|\Delta\mathbf{X}_j\|_F \leq \delta_j \|\mathbf{X}_j\|_2$  for all  $j$ , then

$$\left\| \prod_{j=1}^n (\mathbf{X}_j + \Delta\mathbf{X}_j) - \prod_{j=1}^n \mathbf{X}_j \right\|_F \leq \left( -1 + \prod_{j=1}^n (1 + \delta_j) \right) \prod_{j=1}^n \|\mathbf{X}_j\|_2.$$

LEMMA 3.4. Consider applying a sequence of transformations  $\mathbf{Q} = \mathbf{P}_r \cdots \mathbf{P}_2 \mathbf{P}_1$  onto vector  $\mathbf{x} \in \mathbb{R}^m$  to form  $\hat{\mathbf{y}} = \text{fl}(\hat{\mathbf{P}}_r \cdots \hat{\mathbf{P}}_2 \hat{\mathbf{P}}_1 \mathbf{x})$ , where  $\hat{\mathbf{P}}_k$ 's are Householder transformations constructed from  $\hat{\beta}_k$  and  $\hat{\mathbf{v}}_k$ . These Householder vectors and constants are computed via [alg. 2](#) and the rounding errors are bounded by (3.4) and (3.7). If each transformation is computed via (3.8), then

$$(3.13) \quad \hat{\mathbf{y}} = \mathbf{Q}(\mathbf{x} + \Delta\mathbf{x}) = (\mathbf{Q} + \Delta\mathbf{Q})\mathbf{x},$$

$$(3.14) \quad \|\Delta\mathbf{y}\|_2 \leq r\tilde{\gamma}_m\|\mathbf{x}\|_2, \quad \|\Delta\mathbf{Q}\|_F \leq r\tilde{\gamma}_m.$$

320 *Proof.* Applying [Lemma 3.3](#) directly to  $\mathbf{Q}$  yields

$$321 \quad \|\hat{\mathbf{Q}} - \mathbf{Q}\|_F = \left\| \prod_{j=1}^r (\mathbf{P}_j + \Delta\mathbf{P}_j) - \prod_{j=1}^r \mathbf{P}_j \right\|_F \leq (1 + \tilde{\gamma}_m)^r - 1 \prod_{j=1}^n \|\mathbf{P}_j\|_2 \leq (1 + \tilde{\gamma}_m)^r - 1$$

323 since  $\mathbf{P}_j$ 's are orthogonal and have 2-norm, 1. While we omit the details here, we can show that  
 324  $(1 + \tilde{\gamma}_m)^r - 1 \leq r\tilde{\gamma}_m$  using the argument for [Lemma 2.1](#) if  $r\tilde{\gamma}_m \leq 1/2$ .  $\square$

325 In this current uniform precision error analysis, the important quantity  $\tilde{\gamma}_m$  is derived from the back-  
 326 ward error of applying one Householder transformation. To easily generalize this section for mixed  
 327 precision analysis, we benefit from alternatively denoting this quantity as  $\tilde{\gamma}_{\mathbf{P}}$  with the understand-  
 328 ing that  $\tilde{\gamma}_{\mathbf{P}}$  will be some combination of  $\tilde{\gamma}$ 's of differing precisions. The bound in [Equation \(3.14\)](#)  
 329 would then be replaced by  $r\tilde{\gamma}_{\mathbf{P}}$ . Applying [Lemma 3.2](#) directly to columns of  $\mathbf{A}$  and  $\mathbf{I}$  allows us  
 330 to formulate 2-norm forward bounds for columns of  $\mathbf{R}$  and  $\mathbf{Q}$ . We show how to convert these  
 331 columnwise bounds into matrix norms for the  $\mathbf{R}$  factor.

$$332 \quad \|\Delta\mathbf{R}\|_F = \left( \sum_{i=1}^n \|\Delta\mathbf{R}[:, i]\|_2^2 \right)^{1/2} \leq \left( \sum_{i=1}^n n^2 \tilde{\gamma}_m^2 \|\mathbf{A}[:, i]\|_2^2 \right)^{1/2} = n\tilde{\gamma}_m \|\mathbf{A}\|_F,$$

333  
 334 We gather these results into [Theorem 3.5](#).

335 **THEOREM 3.5.** *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  
 337 the thin QR factors of  $\mathbf{A}$  obtained via [alg. 3](#). Then,*

$$338 \quad \hat{\mathbf{R}} = \mathbf{R} + \Delta\mathbf{R} = \mathbf{fl}(\hat{\mathbf{P}}_n \cdots \hat{\mathbf{P}}_1 \mathbf{A}), \quad \|\Delta\mathbf{R}[:, j]\|_2 \leq n\tilde{\gamma}_m \|\mathbf{A}[:, j]\|_2, \quad \|\Delta\mathbf{R}\|_F \leq n\tilde{\gamma}_m \|\mathbf{A}\|_F$$

$$339 \quad \hat{\mathbf{Q}} = \mathbf{Q} + \Delta\mathbf{Q} = \mathbf{fl}(\hat{\mathbf{P}}_1 \cdots \hat{\mathbf{P}}_n \mathbf{I}), \quad \|\Delta\mathbf{Q}[:, j]\|_2 \leq n\tilde{\gamma}_m, \quad \|\Delta\mathbf{Q}\|_F \leq n^{3/2}\tilde{\gamma}_m.$$

341 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 e—rror is

$$342 \quad (3.15) \quad \|\Delta\mathbf{A}\|_F \leq n^{3/2}\tilde{\gamma}_m \|\mathbf{A}\|_F.$$

343 For the remainder of this paper, we compare various QR factorizations with respect to  $\|\hat{\mathbf{Q}} - \mathbf{Q}\|_F$ , a  
 344 comprehensive measure of orthogonality of the  $\mathbf{Q}$  factor. The content of this section generalizes the  
 345 standard rounding error analysis in [\[12\]](#) by employing quantities denoted via  $\Delta\beta$ ,  $\Delta\mathbf{v}$ ,  $\tilde{\gamma}_y$ , and  $\tilde{\gamma}_{\mathbf{P}}$ .  
 346 These quantities account for various forward and backward errors formed in computing essential  
 347 components of HQR, namely the Householder constant and vector, as well as normwise errors of the  
 348 action of applying Householder transformations. In the next sections, we present blocked variants  
 349 of HQR that use [alg. 3](#).

350 **3.2. Block HQR with partitioned columns (BQR).** We refer to the blocked variant  
 351 of HQR where the columns are partitioned as BQR. Note that this algorithm relies on the WY  
 352 representation described in [\[4\]](#) instead of the storage-efficient version of [\[19\]](#).

353 **3.2.1. The WY Representation.** A convenient matrix representation that accumulates  $r$   
 354 Householder reflectors is known as the WY representation (see [\[4, 9\]](#)). [Lemma 3.6](#) shows how to  
 355 update a rank- $j$  update of the identity,  $\mathbf{Q}^{(j)}$ , with a Householder transformation,  $\mathbf{P}$ , to produce a  
 356 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. This algorithm assumes that the Householder vectors,  $\mathbf{V}$ , and constants,  $\beta$ , have already been computed. Since the  $\mathbf{Y}$  factor is exactly  $\mathbf{V}$ , we only need to compute the  $\mathbf{W}$  factor.

LEMMA 3.6. 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:**  $\mathbf{W}, \mathbf{Y} \leftarrow \text{buildWY}(\mathbf{V}, \beta)$ : 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:**  $\mathbf{W}$

```

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

---

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  $k^{\text{th}}$  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  $k^{\text{th}}$  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  $k^{\text{th}}$  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 [9]), 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 standard precision. A pseudoalgorithm for BQR is shown in alg. 5. Note that the subscripts on  $\mathbf{W}_i$  indicate the WY representation for the Householder transformations on the  $i^{\text{th}}$  block of  $\mathbf{A}$ ,  $\mathbf{C}_k$ , whereas the superscripts on  $\mathbf{W}^{(j)}$  in Lemma 3.6 refers to the  $j^{\text{th}}$  update within building a WY representation.

**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  $\mathbf{W}$  factor, and 3) updating the

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**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    $\mathbf{W}_i \leftarrow \text{buildWY}(\mathbf{V}_i, \beta_i)$                                    /* Algorithm 4 */
5    $[\mathbf{C}_{i+1} \cdots \mathbf{C}_N] \leftarrow \mathbf{V}_i (\mathbf{W}_i^\top [\mathbf{C}_{i+1} \cdots \mathbf{C}_N])$  /* 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.
6  $\mathbf{Q} \leftarrow \mathbf{I}$                                                          /*  $\mathbf{I}_m$  if full QR, and  $\mathbf{I}_{m \times n}$  if thin QR. */
7 for  $i = N : -1 : 1$  do
8    $\mathbf{Q}[(i-1)r+1 : m, (i-1)r+1 : n] \leftarrow \mathbf{W}_i (\mathbf{V}_i^\top \mathbf{Q}[(i-1)r+1 : m, (i-1)r+1 : n])$ 
9 return  $\mathbf{Q}, \mathbf{A}$ 
```

---

387 remaining blocks with the WY representation. We have adapted the analysis from [12] to fit this  
 388 exact variant. Furthermore, we assume that  $n$  is divisible by  $r$  so that  $N = \lceil n/r \rceil = n/r$  to make  
 389 our error analysis simple. In practice, an efficient implementation might require  $r$  to be a power of  
 390 two or a product of small prime factors and result a thinner  $N^{\text{th}}$  block compared to the rest. This  
 391 discrepancy is easily fixed by padding the matrix with zeros, a standard procedure for standard  
 392 algorithms like the Fast Fourier Transform (FT).

393 *HQR within each block: line 3 of alg. 5.* We apply Algorithm 3 to the  $k^{\text{th}}$  block,  $\mathbf{C}_k$ , which is  
 394 equivalent to  $r$  Householder transformations of size  $m - (r-1)k$  under the assumption that  $n = Nr$ .  
 395 A normwise bound for the  $\mathbf{R}$  factor of  $\mathbf{C}_k$  can be easily adapted from Theorem 3.5.

*Build WY at each block: line 4 of alg. 5.* We now calculate the rounding errors incurred from  
 building the WY representation when given a set of Householder vectors and constants as shown  
 in alg. 4. Our goal is to analyze the error accumulated from updating the WY representation from  
 the  $j-1^{\text{st}}$  step to the  $j^{\text{th}}$  for block  $\mathbf{C}_k$ . Let us represent the  $j^{\text{th}}$  Householder constant and vector  
 of the  $k^{\text{th}}$  block computed with FLOPs as with  $\hat{\beta}_k^{(j)}$  and  $\hat{\mathbf{v}}_k^{(j)}$  and the  $j'^{\text{th}}$  update to the WY  
 representation as

$$\mathbf{X}_k^{(j')} = \mathbf{I} - \hat{\mathbf{W}}_k^{(j')} \hat{\mathbf{Y}}_k^{(j')\top}.$$

396 The update in Lemma 3.6 applies a rank-1 update via the subtraction of the outer product  $\hat{\mathbf{z}}_k^{(j)} \hat{\mathbf{v}}_k^{(j)\top}$   
 397 to apply  $\hat{\mathbf{P}}_{(k-1)r+j}$  on the right. Since  $\mathbf{z}_k^{(j)} = \beta_k^j \mathbf{X}_k^{(j-1)} \mathbf{v}_k^{(j)}$ , this update requires a single Householder  
 398 transformation in the same efficient implementation that is discussed in Lemma 3.2, but on the right  
 399 side:

$$\begin{aligned}
 400 \quad \mathbf{X}_k^{(j)} &= \mathbf{X}_k^{(j-1)} - \beta_k^j \mathbf{X}_k^{(j-1)} \mathbf{v}_k^{(j)} \mathbf{v}_k^{(j-1)\top} \\
 401 \quad &= \mathbf{X}_k^{(j-1)} (\mathbf{I} - \beta_k^{(j)} \mathbf{v}_k^{(j)} \mathbf{v}_k^{(j-1)\top}) = \mathbf{X}_k^{(j-1)} \mathbf{P}_{(k-1)r+j}.
 \end{aligned}$$

403 Traveling up this recursion relation to  $j = 1$ , we find that  $\hat{\mathbf{X}}_k^{(j')}$  is built from applying a sequence  
 404 of Householder transformations  $\{\hat{\mathbf{P}}_{(k-1)r+1}, \dots, \hat{\mathbf{P}}_{(k-1)r+j'-1}\}$  to  $\mathbf{I}$ . Therefore, we can apply (3.14)

(set  $\mathbf{Q} = \mathbf{X}_k^{(j-1)}$ ,  $\mathbf{x} = \text{fl}(\hat{\beta}_k^{(j)} \hat{\mathbf{v}}_k^{(j)})$ , and  $\mathbf{y} = \mathbf{z}_k^{(j)}$ ) to form (3.16). More details on the WY update is summarized in Lemma 3.7.

LEMMA 3.7. Consider the construction of the WY representation for the  $k^{\text{th}}$  partition of matrix  $\mathbf{A}^{m \times n}$  given a set of Householder constants and vectors,  $\{\beta_k^{(j)}\}_{j=1}^r$  and  $\{\mathbf{v}_k^{(j)}\}$  via alg. 4. Then,

$$(3.16) \quad \hat{\mathbf{z}}_k^{(j)} = \mathbf{z}_k^{(j)} + \Delta \mathbf{z}_k^{(j)}, \quad |\Delta \mathbf{z}_k^{(j)}| \leq j \tilde{\gamma}_{m-(k-1)r} |\mathbf{z}_k^{(j)}|$$

$$(3.17) \quad \hat{\mathbf{v}}_k^{(j)} = \mathbf{v}_k^{(j)} + \Delta \mathbf{v}_k^{(j)}, \quad |\Delta \mathbf{v}_k^{(j)}| \leq \tilde{\gamma}_{m-(k-1)r} |\mathbf{v}_k^{(j)}|,$$

where the second bound is derived from (3.4).

Most importantly, this shows that constructing the WY update is just as numerically stable as applying successive Householder transformations (see Section 19.5 of [12]).

Update blocks to the right: line 6 of alg. 5. We now consider applying  $\mathbf{X}_k := \mathbf{I} - \mathbf{W}_k \mathbf{Y}_k^\top$  to the bottom right submatrix,  $\mathbf{B} := [\mathbf{C}_{k+1} \cdots \mathbf{C}_N][(k-1)r+1 : m, :]$ . In practice, this step is performed with a level-3 BLAS operation. Regardless, let us analyze the column-wise backward error for the  $j^{\text{th}}$  column of  $\mathbf{B}$ ,  $\mathbf{b}_j$ .

$$\text{fl}(\hat{\mathbf{X}}_k \mathbf{b}_j) = \text{fl}(\mathbf{b}_j - \text{fl}(\hat{\mathbf{W}}_k \text{fl}(\hat{\mathbf{Y}}_k^\top \mathbf{b}_j))) = (1 + \delta)(\mathbf{b}_j - (\hat{\mathbf{W}}_k + \tilde{\Delta} \mathbf{W}_k)(\hat{\mathbf{Y}}_k + \tilde{\Delta} \mathbf{Y}_k)^\top \mathbf{b}_j),$$

where  $\tilde{\Delta} \mathbf{W}_k$  and  $\tilde{\Delta} \mathbf{Y}_k$  each represent the backward error for a matrix-vector multiply with inner products of lengths  $m - (k-1)r$  and  $r$  in level-3 BLAS operations, and  $\hat{\mathbf{W}}_k = \mathbf{W}_k + \Delta \mathbf{W}_k$ ,  $\hat{\mathbf{Y}}_k = \mathbf{Y}_k + \Delta \mathbf{Y}_k$  where the columns of  $\Delta \mathbf{W}_k, \Delta \mathbf{Y}_k$  are bounded by (3.16) and (3.17). If we let  $|\tilde{\Delta} \mathbf{W}_k| \leq \tilde{\gamma}_{\mathbf{W}_k} |\hat{\mathbf{W}}_k|$  and  $|\tilde{\Delta} \mathbf{Y}_k| \leq \tilde{\gamma}_{\mathbf{Y}_k} |\hat{\mathbf{Y}}_k|$ , then we have

$$|\text{fl}(\hat{\mathbf{X}}_k \mathbf{b}_j) - \mathbf{X}_k \mathbf{b}_j| \leq \tilde{\gamma}_{\mathbf{X}_k} \left( |\mathbf{b}_j| + |\hat{\mathbf{W}}_k| |\hat{\mathbf{Y}}_k|^\top |\mathbf{b}_j| \right),$$

where  $\tilde{\gamma}_{\mathbf{X}_k}$  accounts for the errors from perturbations  $\tilde{\Delta} \mathbf{W}_k + \Delta \mathbf{W}_k$ ,  $\tilde{\Delta} \mathbf{Y}_k + \Delta \mathbf{Y}_k$ , and  $\delta$ . In uniform precision, this is largely derived from

$$\begin{aligned} & |(\mathbf{W}_k + \Delta \mathbf{W}_k + \tilde{\Delta} \mathbf{W}_k)(\mathbf{Y}_k + \Delta \mathbf{Y}_k + \tilde{\Delta} \mathbf{Y}_k)^\top \mathbf{b}_j - \mathbf{W}_k \mathbf{Y}_k^\top \mathbf{b}_j| \\ & \leq [(1 + r \tilde{\gamma}_{m-(k-1)r} + \gamma_r)(1 + \tilde{\gamma}_{m-(k-1)r} + \gamma_{m-(k-1)r}) - 1] |\mathbf{W}_k| |\mathbf{Y}_k|^\top |\mathbf{b}_j| \\ & \leq r \tilde{\gamma}_{m-(k-1)r} |\mathbf{W}_k| |\mathbf{Y}_k|^\top |\mathbf{b}_j|, \quad \gamma_{\mathbf{X}_k} := r \tilde{\gamma}_{m-(k-1)r}, \end{aligned}$$

since the subtraction step only adds a single rounding error. We conclude with a general bound,

$$(3.18) \quad \text{fl}(\hat{\mathbf{X}}_k \mathbf{b}_j) = (\mathbf{X}_k + \Delta \mathbf{X}_k) \mathbf{b}_j, \quad \|\Delta \mathbf{X}_k\|_F \leq \tilde{\gamma}_{\mathbf{X}_k},$$

where  $\tilde{\gamma}_{\mathbf{X}_k} = r \tilde{\gamma}_{m-(k-1)r}$  in uniform precision. A normwise bound for a general matrix-matrix multiplication operation is stated in section 19.5 of [12].

Multiple WY updates: line 8-9 of alg. 5. All that remains is to consider the application of successive WY updates to form the QR factorization computed with BQR denoted as  $\mathbf{Q}_{BQR}$  and  $\mathbf{R}_{BQR}$ . We can apply Lemma 3.3 directly by setting  $\mathbf{X}_k := \mathbf{I} - \mathbf{W}_k \mathbf{Y}_k^\top$  and consider the backward errors for applying the sequence to a vector,  $\mathbf{x} \in \mathbb{R}^m$ , as we did for Lemma 3.4. Since  $\mathbf{X}_k = \mathbf{P}_{(k-1)r+1} \cdots \mathbf{P}_{kr}$ , is simply a sequence of Householder transformations, it is orthogonal, i.e.  $\|\mathbf{X}_k\|_2 = 1$ . We only need to replace with  $\mathbf{x}$  with  $\mathbf{A}[:, i]$ 's to form the columnwise bounds for  $\mathbf{R}_{BQR}$ ,



442 and apply the transpose to  $\hat{e}_i$ 's to form the bounds for  $\mathbf{Q}_{BQR}$ . Then,

$$443 \quad (3.19) \quad \left\| \prod_{k=1}^N (\mathbf{X}_k + \Delta \mathbf{X}_k) - \prod_{k=1}^N \mathbf{X}_k \right\|_F \leq \sum_{k=1}^N (1 + \tilde{\gamma}_{\mathbf{X}_k}) - 1 \leq rN\tilde{\gamma}_m \equiv n\tilde{\gamma}_m,$$

$$444 \quad (3.20) \quad \|\hat{\mathbf{Q}}_{BQR} - \mathbf{Q}\|_F \leq n^{3/2}\tilde{\gamma}_m.$$

446 We showed earlier in this section that HQR performed on  $\mathbf{C}_k$  accrues error of order  $\tilde{\gamma}_{m-(k-1)r}$  by  
 447 applying creftm:feHQR, and the building of the  $\mathbf{W}$  factor,  $r\tilde{\gamma}_{m-(k-1)r}$  order error. Both of these  
 448 are relatively small in comparison to the error from applying many WY transformations, so we  
 449 attribute the leading order error to this last step shown in (3.20). The primary goal of the analysis  
 450 presented in this section is to make the generalization to mixed precision settings in section 4 easier,  
 451 and readers should refer to [9, 12] for full details.

452 **3.3. Block HQR with partitioned rows : Tall-and-Skinny QR (TSQR).** Some im-  
 453 portant problems that require QR factorizations of overdetermined systems include least squares  
 454 problems, eigenvalue problems, low rank approximations, as well as other matrix decompositions.  
 455 Although Tall-and-Skinny QR (TSQR) broadly refers to block QR factorization methods with row  
 456 partitions, we will discuss a specific variant of TSQR which is also known as the AllReduce algo-  
 457 rithm [18]. In this paper, the TSQR/AllReduce algorithm refers to the most parallel variant of  
 458 the block QR factorization algorithms discussed in [8]. A detailed description and rounding error  
 459 analysis of this algorithm can be found in [18], and we present a pseudocode for the algorithm in  
 460 alg. 6. Our initial interest in this algorithm came from its parallelizable nature, which is particu-  
 461 larly suitable to implementation on GPUs. Additionally, our numerical simulations (discussed in  
 462 section 5) show that TSQR can not only increase the speed but also outperform the traditional  
 463 HQR factorization in low precisions.

464 **3.3.1. TSQR/AllReduce Algorithm.** Algorithm 6 partitions the rows of a tall-and-skinny  
 465 matrix,  $\mathbf{A}$ . HQR is performed on each of those blocks and pairs of  $\mathbf{R}$  factors are combined to form  
 466 the next set of  $\mathbf{A}$  matrices to be QR factorized. This process is repeated until only a single  $\mathbf{R}$  factor  
 467 remains, and the  $\mathbf{Q}$  factor is built from all of the Householder constants and vectors stored at each  
 468 level. The most gains from parallelization can be made in the initial level where the maximum  
 469 number of independent HQR factorizations occur. Although more than one configuration of this  
 470 algorithm may be available for a given tall-and-skinny matrix, the number of nodes available and  
 471 the shape of the matrix eliminate some of those choices. For example, a 1600-by-100 matrix can  
 472 be partitioned into 2, 4, 8, or 16 initial row-blocks but may be restricted by a machine with only  
 473 4 nodes, and a 1600-by-700 matrix can only be partitioned into 2 initial blocks. Our numerical  
 474 experiments show that the choice in the initial partition, which directly relates to the recursion  
 475 depth of TSQR, has an impact in the accuracy of the QR factorization.

476 We refer to *level* as the number of recursions in a particular TSQR implementation. An  $L$ -level  
 477 TSQR algorithm partitions the original matrix into  $2^{(l)}$  submatrices in the initial or  $0^{th}$  level of the  
 478 algorithm, and  $2^{L-i}$  QR factorizations are performed in level  $i$  for  $i = 1, \dots, L$ . The set of matrices  
 479 that are QR factorized at each level  $i$  are called  $\mathbf{A}_j^{(i)}$  for  $j = 1, \dots, 2^{L-i}$ , where superscript  $(i)$   
 480 corresponds to the level and the subscript  $j$  indexes the row-blocks within level  $i$ . In the following  
 481 sections, alg. 6 (tsqr) will find a TSQR factorization of a matrix  $A \in \mathbb{R}^{m \times n}$  where  $m \gg n$ . The  
 482 inline function `qr` refers to alg. 3 and we use alg. 2 as a subroutine of `qr`.

483 *TSQR Notation.* We introduce new notation due to the multi-level nature of the TSQR algo-  
 484 rithm. In the final task of constructing  $\mathbf{Q}$ ,  $\mathbf{Q}_j^{(i)}$  factors are aggregated from each block at each level.



Each  $\mathbf{Q}_j^{(i)}$  factor from level  $i$  is partitioned such that two corresponding  $\mathbf{Q}^{(i-1)}$  factors from level  $i-1$  can be applied to them. The partition (approximately) splits  $\mathbf{Q}_j^{(i)}$  into two halves,  $[\tilde{\mathbf{Q}}_{j,1}^{(i)\top} \tilde{\mathbf{Q}}_{j,2}^{(i)\top}]^\top$ . The functions  $\alpha(j)$  and  $\phi(j)$  are defined such that  $\mathbf{Q}_j^{(i)}$  is applied to the correct blocks from the level below:  $\tilde{\mathbf{Q}}_{\alpha(j),\phi(j)}^{(i+1)}$ . For  $j = 1, \dots, 2^{L-i}$  at level  $i$ , we need  $j = 2(\alpha(j) - 1) + \phi(j)$ , where  $\alpha(j) = \lceil \frac{j}{2} \rceil$  and  $\phi(j) = 2 + j - 2\alpha(j) \in \{1, 2\}$ . [section 3.3.2](#) shows full linear algebra details for a single-level ( $L = 1, 2$  initial blocks) example. The reconstruction of  $\mathbf{Q}$  can be implemented more efficiently (see [\[3\]](#)), but the reconstruction method in [alg. 6](#) is presented for a clear, straightforward explanation.

**3.3.2. Single-level Example.** In the single-level version of this algorithm, we first bisect  $\mathbf{A}$  into  $\mathbf{A}_1^{(0)}$  and  $\mathbf{A}_2^{(0)}$  and compute the QR factorization of each of those submatrices. We combine the resulting upper-triangular matrices (see below) which is QR factorized, and the process is repeated:

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_1^{(0)} \\ \mathbf{A}_2^{(0)} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1^{(0)} \mathbf{R}_1^{(0)} \\ \mathbf{Q}_2^{(0)} \mathbf{R}_2^{(0)} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \begin{bmatrix} \mathbf{R}_1^{(0)} \\ \mathbf{R}_2^{(0)} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \mathbf{A}_1^{(1)} = \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \mathbf{Q}_1^{(1)} \mathbf{R}.$$

The  $\mathbf{R}$  factor of  $\mathbf{A}_1^{(1)}$  is the final  $\mathbf{R}$  factor of the QR factorization of the original matrix,  $\mathbf{A}$ . However, the final  $\mathbf{Q}$  still needs to be constructed. Bisecting  $\mathbf{Q}_1^{(1)}$  into two submatrices, i.e.  $\tilde{\mathbf{Q}}_{1,1}^{(1)}$  and  $\tilde{\mathbf{Q}}_{1,2}^{(1)}$ , allows us to write and compute the product more compactly,

$$\mathbf{Q} := \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \mathbf{Q}_1^{(1)} = \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{Q}}_{1,1}^{(1)} \\ \tilde{\mathbf{Q}}_{1,2}^{(1)} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1^{(0)} \tilde{\mathbf{Q}}_{1,1}^{(1)} \\ \mathbf{Q}_2^{(0)} \tilde{\mathbf{Q}}_{1,2}^{(1)} \end{bmatrix}.$$

More generally, [alg. 6](#) takes a tall-and-skinny matrix  $\mathbf{A}$  and level  $L$  and finds a QR factorization by initially partitioning  $\mathbf{A}$  into  $2^{(l)}$  row-blocks and includes the building of  $\mathbf{Q}$ . For simplicity, we assume that  $m$  is exactly  $h2^{(l)}$  so that the initial partition yields  $2^{(l)}$  blocks of equal sizes,  $h$ -by- $n$ . Also, note that `hh_mult` refers to the action of applying multiple Householder transformations given a set of Householder vectors and constants, which can be performed by iterating line 6 of [alg. 3](#). This step can be done in a level-3 BLAS operation via a WY update if [alg. 6](#) was modified to store the WY representation at the QR factorization of each block of each level,  $\mathbf{A}_j^{(i)}$ .

**3.3.3. TSQR: Rounding Error Analysis.** The TSQR algorithm presented in [alg. 6](#) is a divide-and-conquer strategy for the QR factorization that uses the HQR within the subproblems. Divide-and-conquer methods can naturally be implemented in parallel and accumulate less rounding errors. For example, the single-level TSQR decomposition of a tall-and-skinny matrix,  $\mathbf{A}$  requires 3 total HQRs of matrices of sizes  $\lfloor \log_2(\frac{m}{n}) \rfloor$ -by- $n$ ,  $\lfloor \log_2(\frac{m}{n}) \rfloor$ -by- $n$ , and  $2n$ -by- $n$ . The single-level TSQR strictly uses more FLOPs, but the dot product subroutines may accumulate smaller rounding errors (and certainly have smaller upper bounds) since they are performed on shorter vectors, and lead to a more accurate solution overall. These concepts are elucidated in [\[18\]](#), where the rounding error analysis of TSQR is shown in detail in [\[18\]](#). We summarize the main results from [\[18\]](#) in

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**Algorithm 6:  $\mathbf{Q}, \mathbf{R} = \text{tsqr}(\mathbf{A}, L)$ .** Finds a QR factorization of a tall, skinny matrix,  $\mathbf{A}$ .

---

**Input:**  $\mathbf{A} \in \mathbb{R}^{m \times n}$  where  $m \gg n$ ,  $L \leq \lfloor \log_2 \left( \frac{m}{n} \right) \rfloor$ , and  $2^L$  is the initial number of blocks.  
**Output:**  $\mathbf{Q} \in \mathbb{R}^{m \times n}$ ,  $\mathbf{R} \in \mathbb{R}^{n \times n}$  such that  $\mathbf{QR} = \mathbf{A}$ .

```

1  $h \leftarrow m2^{-L}$  // Number of rows.
  /* Split  $\mathbf{A}$  into  $2^L$  blocks. Note that level  $(i)$  has  $2^{L-i}$  blocks. */
2 for  $j = 1 : 2^L$  do
3    $\mathbf{A}_j^{(0)} \leftarrow \mathbf{A}[(j-1)h + 1 : jh, :]$ 
  /* Store Householder vectors as columns of matrix  $\mathbf{V}_j^{(i)}$ , Householder
     constants as components of vector  $\beta_j^{(i)}$ , and set up the next level. */
4 for  $i = 0 : L - 1$  do
5   /* The inner loop can be parallelized. */
6   for  $j = 1 : 2^{L-i}$  do
7      $\mathbf{V}_{2j-1}^{(i)}, \beta_{2j-1}^{(i)}, \mathbf{R}_{2j-1}^{(i)} \leftarrow \text{qr}(\mathbf{A}_{2j-1}^{(i)})$ 
8      $\mathbf{V}_{2j}^{(i)}, \beta_{2j}^{(i)}, \mathbf{R}_{2j}^{(i)} \leftarrow \text{qr}(\mathbf{A}_{2j}^{(i)})$ 
9      $\mathbf{A}_j^{(i+1)} \leftarrow \begin{bmatrix} \mathbf{R}_{2j-1}^{(i)} \\ \mathbf{R}_{2j}^{(i)} \end{bmatrix}$ 
10   $\mathbf{V}_1^{(L)}, \beta_1^{(L)}, \mathbf{R} \leftarrow \text{qr}(\mathbf{A}_1^{(L)})$  // The final  $\mathbf{R}$  factor is built.
11   $\mathbf{Q}_1^{(L)} \leftarrow \text{hh\_mult}(\mathbf{V}_1^{(L)}, I_{2n \times n})$ 
12  /* Compute  $\mathbf{Q}^{(i)}$  factors by applying  $\mathbf{V}^{(i)}$  to  $\mathbf{Q}^{(i+1)}$  factors. */
13 for  $i = L - 1 : -1 : 1$  do
14   for  $j = 1 : 2^{L-i}$  do
15      $\mathbf{Q}_j^{(i)} \leftarrow \text{hh\_mult} \left( \mathbf{V}_j^{(i)}, \begin{bmatrix} \tilde{\mathbf{Q}}_{\alpha(j), \phi(j)}^{(i+1)} \\ \mathbf{0} \end{bmatrix} \right)$ 
16  $\mathbf{Q} \leftarrow []$ ; // Construct the final  $\mathbf{Q}$  factor.
17 for  $j = 1 : 2^L$  do
18    $\mathbf{Q} \leftarrow \begin{bmatrix} \mathbf{Q} \\ \text{hh\_mult} \left( \mathbf{V}_j^{(0)}, \begin{bmatrix} \tilde{\mathbf{Q}}_{\alpha(j), \phi(j)}^{(1)} \\ \mathbf{0} \end{bmatrix} \right) \end{bmatrix}$ 
19 return  $\mathbf{Q}, \mathbf{R}$ 
```

---

THEOREM 3.8. Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with  $m \geq n$  have full rank,  $n$ , and  $\hat{\mathbf{Q}} \in \mathbb{R}^{m \times n}$  and  $\hat{\mathbf{R}} \in \mathbb{R}^{n \times n}$  be the thin QR factors of  $\mathbf{A}$  obtained via [alg. 6](#) with  $L$  levels. Let us further assume that  $m = h2^{(l)}$  and  $n\tilde{\gamma}_{m2^{-L}}, n\tilde{\gamma}_{2n} \ll 1$ . Then, normwise error bounds for the  $j^{\text{th}}$  column ( $j = 1 : n$ ) are

$$(3.21) \quad \|\hat{\mathbf{R}}_{TSQR}[:, j] - \mathbf{R}[:, j]\|_2 \leq n(\tilde{\gamma}_{m2^{-L}} + L\tilde{\gamma}_{2n})\|\mathbf{A}[:, j]\|_2,$$

$$(3.22) \quad \|\hat{\mathbf{Q}}_{TSQR}[:, j] - \mathbf{Q}[:, j]\|_2 \leq n(\tilde{\gamma}_{m2^{-L}} + L\tilde{\gamma}_{2n}).$$

Note that the  $n\tilde{\gamma}_{m2^{-L}}$  and  $n\tilde{\gamma}_{2n}$  terms correspond to errors from applying HQR to the blocks in the initial partition and to the blocks in levels 1 through  $L$  respectively. We can easily replace

these with analogous mixed precision terms and keep the analysis accurate. Both level-2 and level-3 BLAS implementations will be considered in [section 4](#).

**4. Mixed precision error analysis.** Let us first consider rounding errors incurred from carrying out HQR in high precision, then cast down at the very end. This could be useful in applications that require economical storage but have enough memory to carry out HQR in higher precision, or in block algorithms as will be shown in [subsections 4.1](#) and [4.2](#). Consider two floating point types  $\mathbb{F}_{low}$  and  $\mathbb{F}_{high}$  where  $\mathbb{F}_l \subseteq \mathbb{F}_h$ , and for all  $x, y \in \mathbb{F}_l$ , the exact product  $xy$  can be represented in  $\mathbb{F}_h$ . Some example pairs of  $\{\mathbb{F}_l, \mathbb{F}_h\}$  include  $\{\text{fp16}, \text{fp32}\}$ ,  $\{\text{fp32}, \text{fp64}\}$ , and  $\{\text{fp16}, \text{fp64}\}$ . Suppose that the matrix to be factorized is stored with low precision numbers,  $\mathbf{A} \in \mathbb{F}_l^{m \times n}$ . Casting up adds no rounding errors, so we can directly apply the analysis that culminated in [Theorem 3.5](#), and we only consider the columnwise forward error in the  $\mathbf{Q}$  factor. Then, the  $j^{th}$  column of  $\hat{\mathbf{Q}}_{HQR} = \mathbf{Q} + \Delta\mathbf{Q}_{HQR}$  is bounded normwise via  $\|\Delta\mathbf{Q}_{HQR}[:, j]\|_2 \leq n\tilde{\gamma}_m^{high}$ , and incurs an extra rounding error when  $\mathbf{Q} \in \mathbb{F}_{high}^{m \times n}$  is cast down to  $\mathbb{F}_{low}^{m \times n}$ . Consider the backward error of a cast down operation represented by a linear transformation,

First, consider casting down a vector  $\mathbf{x}^{(h)} \in \mathbb{F}_h^m$  to  $\mathbb{F}_l^m$ . We see that

$$(4.1) \quad \mathbf{x}^{(l)} := \text{castdown}(\mathbf{x}^{(h)}) = \mathbf{I}_l \mathbf{x}^{(h)} = (\mathbf{I} + \mathbf{E}) \mathbf{x}^{(h)} = \mathbf{x}^{(h)} + \Delta\mathbf{x},$$

where  $|\Delta\mathbf{x}| \leq u^{(l)} |\mathbf{x}^{(h)}|$  and  $\|\Delta\mathbf{x}\|_2 \leq u^{(l)} \|\mathbf{x}^{(h)}\|_2$ . Then,  $\mathbf{E} = \Delta\mathbf{x}\mathbf{x}^\top / \|\mathbf{x}\|_2^2$  and we can use the same argument as in [\(3.11\)](#) to form a backward matrix norm bound,

$$(4.2) \quad \|\mathbf{E}\|_F \leq u^{(l)}.$$

Using this in [Lemma 3.3](#) to analyze the forward norm error for the  $j^{th}$  column of the  $\mathbf{Q}$  factor computed with [alg. 3](#) yields

$$(4.3) \quad \|\text{castdown}(\hat{\mathbf{Q}}_{HQR}[:, j]) - \mathbf{Q}[:, j]\|_2 = \|\mathbf{I}_l \hat{\mathbf{P}}_1 \cdots \hat{\mathbf{P}}_n \hat{\mathbf{e}}_j\|_2 \leq u^{(l)} + n\tilde{\gamma}_m^{(h)}.$$

To convert this bound to the lower precision, we define function  $d$ ,

$$(4.4) \quad d(m, u^{(h)}, q, u^{(l)}) := \lceil (qu^{(l)} + mu^{(h)})/u^{(l)} \rceil = \mathcal{O}(q + mu^{(h)}/u^{(l)}),$$

so that if  $\|\hat{\mathbf{x}} - \mathbf{x}\|_2 \leq \gamma_m^{(h)}$ , then  $\|\text{castdown}(\hat{\mathbf{x}}) - \mathbf{x}\|_2 \leq \gamma_{d(m, u^{(h)}, q, u^{(l)})}^{(l)}$ . This is a looser bound but it allows us to easily compare the errors to the uniform, low precision implementation of forming  $\hat{\mathbf{x}}$ .

We can easily apply the operator  $\mathbf{I}^{(l)}$  to cast down the QR factorizations computed via BQR and TSQR to find the forward matrix norm error on the  $\mathbf{Q}$  factor as shown below,

$$\begin{aligned} \|\hat{\mathbf{Q}}_{BQR}\|_F &\leq u^{(l)} + n\tilde{\gamma}_m^{(h)} \leq \tilde{\gamma}_{d(nm, u^{(h)}, u^{(l)})}^{(l)}, \\ \|\hat{\mathbf{Q}}_{TSQR}\|_F &\leq u^{(l)} + n(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2-L}^{(h)}) \leq \tilde{\gamma}_{d(n(L2n+m2-L), u^{(h)}, 1, u^{(l)})}^{(l)}. \end{aligned}$$

In the next sections, we consider performing BQR and TSQR with FLOPs within a block and/or a level in high precision, but cast down to low precision in between blocks in [4.1](#). Finally, we consider all 3 algorithms with an ad hoc mixed precision setting where inner products are performed in high precision and all other operations are computed in low precision in [4.2](#).

**4.1. Round down at block-level (BLAS-3).** We use [\(4.3\)](#) to study the errors for BQR and TSQR in the case that each block QR factorized by HQR then cast down.

---

**Algorithm 7:** A portion of a mixed precision BQR: modifying first for-loop in [alg. 5](#).

---

```

1  $q = N/M;$  /* Note that  $n = Nr = qMr$ . */
2 for  $q' = 1 : q$  do
3   if  $q' > 2$  then
4      $\lfloor$  Update  $[\mathbf{C}_{(q'-1)M+1} \cdots \mathbf{C}_{qM}]$  with WY updates from blocks  $1 : (q' - 1)M$ .
5   for  $k = 1 : M$  do
6     Apply HQR to  $\mathbf{C}_{(q'-1)M+k}$ ;
7     Form WY update for  $\mathbf{C}_{(q'-1)M+k}$ ;
8      $\lfloor$  WY update blocks to the right,  $[\mathbf{C}_{(q'-1)M+k+1} \cdots \mathbf{C}_{q'M}]$ .

```

---

**4.1.1. Round down at block level: BQR.** Let us consider a setting in which only  $M$  blocks of width  $r$  can be loaded onto memory. Then, lines 2-6 of [alg. 5](#) can be modified via [alg. 7](#). We now impose a mixed-precision setting where the inner for-loop in [alg. 7](#) is performed in high precision, but the WY updates for the outer loop is stored in low precision and only  $M$  blocks is updated at a time due to the memory constraint. These low precision WY updates would be used to build the  $\mathbf{Q}$  factor serially in groups of  $M$ . Then, the  $j^{\text{th}}$  column of the  $\mathbf{Q}$  factor computed in this mixed-precision BQR algorithm is computed via

$$\hat{\mathbf{Q}}_{mpBQR}[:, j] = \left( \prod_{q'=1}^q (\hat{\mathbf{X}}_{(q'-1)M+1} \cdots \hat{\mathbf{X}}_{q'M} \mathbf{I}^{(l)}) \right) \hat{e}_j.$$

563 Applying [Lemma 3.3](#), we result in bounds

564 (4.5)  $\|\hat{\mathbf{Q}}_{mpBQR}[:, j] - \mathbf{Q}[:, j]\|_2 \leq q(u^{(l)} + Mr\tilde{\gamma}_m^{(h)})$

565 (4.6)  $\|\hat{\mathbf{Q}}_{mpBQR} - \mathbf{Q}\|_F \leq n^{1/2}q(u^{(l)} + Mr\tilde{\gamma}_m^{(h)}),$

567 showing that  $q$  number of cast downs add  $\gamma_q^{(l)}$  order errors to columnwise bounds and the matrix  
568 norm bound is derived from that. This mixed precision BQR variant still rich in level-3 BLAS  
569 operations can be implemented on TensorCore technology. Furthermore, the bounds in (4.5) and  
570 (4.6) show that the loss in precision that can occur from cast downs are linear to the number of  
571 cast downs.

572 **4.1.2. Round down at block level: TSQR.** Let us now consider a WY variant of TSQR,  
573 where all instances of `qr` (lines 6,7,9 of [alg. 6](#)) are followed by `buildWY` (see [alg. 4](#)), and all instances  
574 of `hh_mult` is replaced by a WY update (line 6 of [alg. 5](#)). We additionally impose a mixed precision  
575 assumption similar to [section 4.1.1](#), where we store all WY representations of HQR within the  
576 for-loop (lines 4-8) of [alg. 6](#) in low precision, and consider the construction of the  $\mathbf{Q}$  factor. We can  
577 assume that each  $2n$ -by- $n$  and  $m2^{-L}$ -by- $n$  size matrices can fit into memory and only introduce  
578 one cast down for each  $\mathbf{Q}_j^{(i)}$  block, where  $i = 1 : L - 1$  and  $j = 1 : 2^{i-1}$ . Let us compute lines 9-10  
579 in the higher precision, which introduces an error of order  $n\tilde{\gamma}_{2n}^{(h)}$ . In levels  $L - 1$  to 1, each WY  
580 update adds error  $u^{(l)} + n\tilde{\gamma}_{2n}^{(h)}$ , and the final construction at the  $0^{\text{th}}$  level (line 16), the WY update  
581 adds error  $u^{(l)} + n\tilde{\gamma}_{m2^{-L}}^{(h)}$ . Adding the cast down operator  $\mathbf{I}^{(l)}$  to the analysis in [18] and applying

582 **Lemma 3.3** yields the bounds on  $\hat{\mathbf{Q}}_{mpTSQR}$ ,

$$583 \quad (4.7) \quad \|\hat{\mathbf{Q}}_{mpTSQR}[:, j] - \mathbf{Q}[:, j]\|_2 \leq L(u^{(l)} + n\tilde{\gamma}_{2n}^{(h)}) + \tilde{\gamma}_{m2-L}$$

$$584 \quad (4.8) \quad \|\hat{\mathbf{Q}}_{mpTSQR} - \mathbf{Q}\|_F \leq n^{1/2}(L(u^{(l)} + n\tilde{\gamma}_{2n}^{(h)}) + \tilde{\gamma}_{m2-L}).$$

586 **4.2. Round down at inner-product.** While the previous section discussed blocked variants  
587 of HQR that can be easily adapted for the mixed precision setting specific to TensorCore’s level-3  
588 BLAS operations, we want to provide a more general mixed precision environment in this section.  
589 Recall that HQR, BQR, and TSQR all rely on Householder transformations in one way or another,  
590 and Householder transformations are essentially performed via (3.8). This implementation capital-  
591 izes on the rank-1 update structure of Householder transformations where the predominant share  
592 of FLOPs is spent on an inner product, and computing the Householder vector and constant also  
593 rely heavily on inner products. Therefore, we can attribute nearly all of the computational tasks  
594 for algs. 3, 5 and 6 to the inner product. In addition, the inner product is just as important in  
595 non-HQR linear algebra tools, where some examples include projections and matrix-vector, matrix-  
596 matrix multiply. Consequently, we return to the mixed precision setting described in section 2,  
597 where every inner product is cast down to the lower precision as shown in (2.11).

598 **4.2.1. Round down at inner product: HQR.** Consider forming a Householder transfor-  
599 mation that zeros out  $\mathbf{x} \in \mathbb{R}^m$  below the the  $i^{th}$  element. We need to compute  $\sigma$ ,  $\beta$ ,  $\tilde{\mathbf{v}}_1$ , and  $\mathbf{v}$  as  
600 defined in subsection 3.1:

$$601 \quad (4.9) \quad \text{fl}(\sigma) = \text{fl}(-\text{sign}(\mathbf{x}[1])\|\mathbf{x}\|_2) = \sigma + \Delta\sigma, \quad |\Delta\sigma| \leq (\gamma_2^{(l)} + \gamma_m^{(h)})|\sigma|,$$

$$602 \quad (4.10) \quad \text{fl}(\tilde{\mathbf{v}}_1) = \tilde{\mathbf{v}}_1 + \Delta\tilde{\mathbf{v}}_1 = (1 + \delta^{(l)})(\mathbf{x}_1 - \sigma - \Delta\sigma), \quad |\Delta\tilde{\mathbf{v}}_1| \leq (\gamma_3^{(l)} + \gamma_m^{(h)})|\tilde{\mathbf{v}}_1|$$

$$603 \quad (4.11) \quad \text{fl}(\beta) = \beta + \Delta\beta = (1 + \delta^{(l)}) \left( -\mathbf{v}[1]/\hat{\sigma} \right), \quad |\Delta\beta| \leq (\gamma_4^{(l)} + \tilde{\gamma}_m^{(h)})|\beta|,$$

604  
605

$$606 \quad (4.12) \quad \text{fl}(\mathbf{v}_j) = \mathbf{v}_j + \Delta\mathbf{v}_j \text{ where } |\Delta\mathbf{v}_j| \leq \begin{cases} 0, & j = 1 \\ (\gamma_4^{(l)} + \tilde{\gamma}_m^{(h)})|\mathbf{v}_j|, & j = 2 : m - i + 1. \end{cases}$$

607 Using these, we can formulate the mixed precision version of (3.9) where  $\hat{\mathbf{y}} = \text{fl}(\mathbf{P}_\mathbf{v}\mathbf{x}) \in \mathbb{R}^m$  is  
608 computed with (3.8),

$$609 \quad (4.13) \quad \hat{\mathbf{y}} = \mathbf{y} + \Delta\mathbf{y}, \quad \|\Delta\mathbf{y}\|_2 \leq (\gamma_7^{(l)} + \tilde{\gamma}_m^{(h)})\|\mathbf{y}\|_2.$$

610 Thus, a backward error can be formed using  $\Delta\mathbf{P}_\mathbf{v} = \Delta\mathbf{y}\mathbf{x}^\top / \|\mathbf{x}\|_2^2$ ,

$$611 \quad (4.14) \quad \hat{\mathbf{y}} = (\mathbf{P}_\mathbf{v} + \Delta\mathbf{P}_\mathbf{v})\mathbf{x}, \quad \|\Delta\mathbf{P}_\mathbf{v}\|_F \leq (\gamma_7^{(l)} + \tilde{\gamma}_m^{(h)}).$$

612 The error bounds for applying  $n$  Householder transformations to  $\mathbf{x}$  can be found using Lemma 3.3,

$$613 \quad (4.15) \quad \hat{\mathbf{y}} = \mathbf{Q}(\mathbf{x} + \Delta\mathbf{x}) = (\mathbf{Q} + \Delta\mathbf{Q})\mathbf{x},$$

$$614 \quad (4.16) \quad \|\Delta\mathbf{y}\|_2 \leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)})\|\mathbf{x}\|_2, \quad \|\Delta\mathbf{Q}\|_F \leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}),$$

616 where the leading order error is now  $\mathcal{O}(\gamma_n^{(l)})$ . The analogous mixed precision QR factorization error  
617 bounds are shown in Theorem 4.1.

618 THEOREM 4.1. Let  $\mathbf{A} \in \mathbb{R}^{m \times n}$  with  $m \geq n$  have full rank,  $n$ . Let  $\hat{\mathbf{Q}}_{mpHQR} \in \mathbb{R}^{m \times n}$  and  
619  $\hat{\mathbf{R}} \in \mathbb{R}^{n \times n}_{mpHQR}$  be the thin QR factors of  $\mathbf{A}$  obtained via [alg. 3](#) with mixed precision FLOPs where  
620 inner products are computed in precision  $h$  then cast down. All other operations are carried out in  
621 precision  $l$ . Then,

$$\begin{aligned} 622 \quad \|\Delta \mathbf{R}_{mpHQR}[:, j]\|_2 &\leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}) \|\mathbf{A}[:, j]\|_2, \quad \|\Delta \mathbf{R}_{mpHQR}\|_F \leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}) \|\mathbf{A}\|_F \\ 623 \quad \|\Delta \mathbf{Q}[:, j]_{mpHQR}\|_2 &\leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}), \quad \|\Delta \mathbf{Q}_{mpHQR}\|_F \leq n^{1/2}(\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}). \end{aligned}$$

625 **4.2.2. Round down at inner product: BQR.** Now, we analyze [alg. 5](#) with the same mixed  
626 precision inner product. At the  $k^{th}$  block, we first apply the mixed precision HQR summarized in  
627 [Theorem 4.1](#). Next, we study updating  $\mathbf{W}_k^{j-1}$  to  $\mathbf{W}_k^j$ . Since this update is applied with a single  
628 Householder transformation to the right, we can apply [\(4.16\)](#) to form

$$629 \quad (4.17) \quad \hat{\mathbf{z}}_k^{(j)} = \mathbf{z}_k^{(j)} + \Delta \mathbf{z}_k^{(j)}, \quad |\Delta \mathbf{z}_k^{(j)}| \leq (\tilde{\gamma}_j^{(l)} + j\tilde{\gamma}_{m-(k-1)}^{(h)}) |\mathbf{z}_k^{(j)}|,$$

630 and the error for  $\hat{\mathbf{v}}_k^{(j)}$  is [\(4.12\)](#) with  $m$  replaced by  $m - (k - 1)r$ .

631 **4.2.3. Round down at inner product: TSQR.**

## 632 5. Numerical Experiments.

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

639 The existing rounding error analysis cannot accurately bound the behavior of mixed precision  
640 arithmetic. We have developed a new framework for mixed precision rounding error analysis and  
641 applied it to HQR, a widely used linear algebra routine, and implemented it in an iterative eigen-  
642 solver in the context of spectral clustering. The mixed precision error analysis builds from the  
643 inner product routine, which can be applied to many other linear algebra tools as well. The new  
644 error bounds more accurately describe how rounding errors are accumulated in mixed precision  
645 settings. We also found that TSQR, a communication-avoiding, easily parallelizable QR factor-  
646 ization algorithm for tall-and-skinny matrices, can outperform HQR in mixed precision settings  
647 for ill-conditioned, extremely overdetermined cases, which suggests that some algorithms are more  
648 robust against lower precision arithmetic.

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

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

657

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