ROUNDING ERROR ANALYSIS OF MIXED PRECISION HOUSEHOLDER QR ALGORITHMS

L. MINAH YANG, ALYSON FOX, AND GEOFFREY SANDERS

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) 2-4$\times$ speedup in solving dense large linear equations [10, 11], (ii) 12$\times$ speedup in training dense neural networks, and (iii) 1.2-10$\times$ 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

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

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

This work discusses several aspects of using mixed precision arithmetic: (i) error analysis that can more accurately describe mixed precision arithmetic than existing analyses, (ii) algorithmic design that is more resistant against lower numerical stability associated with lower precision types, and (iii) an example where mixed precision implementation performs as sufficiently as double-precision implementations. Our key findings are that the new mixed precision error analysis produces tighter error bounds, that some block QR algorithms by Demmel et al. [8] are able to operate in low precision more robustly than non-block techniques, and that some small-scale benchmark 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

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

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 *full* QR factorization, whereas a more efficient *thin* QR factorization results in $\mathbf{Q}_1 \in \mathbb{R}^{m \times n}$ and $\mathbf{R}_1 \in \mathbb{R}^{n \times n}$, that is

$$\mathbf{A} = \mathbf{QR} = \begin{bmatrix} \mathbf{Q}_1 & \mathbf{Q}_2 \end{bmatrix} \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{0}_{m-n \times n} \end{bmatrix} = \mathbf{Q}_1 \mathbf{R}_1.$$

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 triangular. In many applications, computing the *thin* decomposition requires less computation and is sufficient in performance. While important definitions are stated explicitly in the text, Table 1 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
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
$\delta^{(q)}$	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

2

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

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

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 [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, $u := \frac{1}{2} b^{1-t}$ in uniform precision settings. In mixed precision settings we denote the higher precision unit round-off with $u^{(h)}$ (h for high) and the lower precision unit round-off with $u^{(l)}$ (l for low).

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 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, $\mathrm{fl}(x \text{ op } y)$, 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:

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

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 $\hat{s_1} := \mathrm{fl}(x + y) = (1 + \delta)(x + y)$, and another rounding error in computing $\hat{s_2} := \mathrm{fl}(\hat{s_1} + z) = (1 + \tilde{\delta})(\hat{s_1} + z)$, where $|\delta|, |\tilde{\delta}| < u$. Then,

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

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.

3

LEMMA 2.1 (Lemma 3.1 [12]). *Let $|\delta_i| < u$ and $\rho_i \in \{-1, +1\}$, for $i = 1, \cdots, k$ and $ku < 1$. Then,*

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

We also use

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

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

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

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

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

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

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

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

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

Although Lemma 2.1 requires $ku < 1$, we actually need $ku < \frac{1}{2}$ to maintain a meaningful relative error bound as this assumption implies $\gamma_k < 1$ and guarantees a relative error below 100%. Since higher precision floating points have smaller unit round-off values, they can tolerate more successive FLOPs than lower precision floating points before reaching $\gamma_m = 1$. Table 3 shows the 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	$\approx$ 4.194e06
FP64	$\approx$ 2.252e15

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

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

4

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

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

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: $\left|\|\mathbf{x}\|_2^2 - \mathrm{fl}(\|\mathbf{x}\|_2^2)\right| \leq \gamma_m \|\mathbf{x}\|_2^2$.
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
$(\gamma_{512}^{\mathrm{fp16}} = 1)$.

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 $\mathrm{fl}(\mathbf{x}^\top \mathbf{y})$ 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

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 com-
puted in simulated half-precision from 2 million realizations.

of vectors sampled from the standard normal distribution have backward relative errors that do not
deviate much from the unit round-off ($\mathcal{O}(\texttt{1e-4})$), whereas the vectors sampled from the uniform
distribution tend to accumulate larger errors on average ($\mathcal{O}(\texttt{1e-3})$). 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 $\texttt{5.466e-2}$ with probability 0.99.

Most importantly, we need error analysis that allows flexibility in precision in order to better
our understanding of the impact of rounding errors on computations done on emerging hardware
(i.e. GPUs) that support mixed precision. 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 θ's and γ's in a *uniform precision* setting.

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.*

5

Algorithm 1: $\mathbf{z}^{(\mathrm{fp16})} = \mathtt{simHalf}(f, \mathbf{x}^{(\mathrm{fp16})}, \mathbf{y}^{(\mathrm{fp16})})$. Simulate function $f \in$ OP$\cup\{\mathtt{dot\_product}\}$ in half precision arithmetic given input variables $\mathbf{x}, \mathbf{y}$. Function $\mathtt{castup}$ converts fp16 to fp32, and $\mathtt{castdown}$ converts fp32 to fp16 by rounding to the nearest half precision float.

Input: $\mathbf{x}^{(\mathrm{fp16})}, \mathbf{y}^{(\mathrm{fp16})} \in \mathbb{F}_{\mathrm{fp16}}^m$, $f : \mathbb{R}^m \times \mathbb{R}^m \to \mathbb{R}^n$

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

1 $\mathbf{x}^{(\mathrm{fp32})}, \mathbf{y}^{(\mathrm{fp32})} \leftarrow \mathtt{castup}([\mathbf{x}^{(\mathrm{fp16})}, \mathbf{y}^{(\mathrm{fp16})}])$

2 $\mathbf{z}^{(\mathrm{fp32})} \leftarrow \mathrm{fl}(f(\mathbf{x}^{(\mathrm{fp32})}, \mathbf{y}^{(\mathrm{fp32})}))$

3 $\mathbf{z}^{(\mathrm{fp16})} \leftarrow \mathtt{castdown}(\mathbf{z}^{(\mathrm{fp32})})$

4 return $\mathbf{z}^{(\mathrm{fp16})}$

---

163 *Arithmetic operations between θ_k's:*

164 (2.8)
$$(1 + \theta_k)(1 + \theta_j) = (1 + \theta_{k+j}) \qquad and \qquad \frac{1 + \theta_k}{1 + \theta_j} = \begin{cases} 1 + \theta_{k+j}, & j \leq k \\ 1 + \theta_{k+2j}, & j > k \end{cases}$$

165 *Operations on γ's:*

166
$$\gamma_k \gamma_j \leq \gamma_{\min(\mathrm{k,j})}, \quad for \ \max_{(\mathrm{j,k})} \mathrm{u} \leq \frac{1}{2},$$

167
$$n\gamma_k \leq \gamma_{nk}, \quad for \quad n \leq \frac{1}{uk},$$

168
$$\gamma_k + u \leq \gamma_{k+1},$$

169
170
$$\gamma_k + \gamma_j + \gamma_k \gamma_j \leq \gamma_{k+j}.$$

171 Let us define a mixed precision setting that is similar to the TensorCore Fused Multiply-Add
172 (FMA) block but works at the level of a dot product. The main difference lies in that the FMA
173 block in TensorCore is for matrix-matrix products (level-3 BLAS) for fp16 and fp32, but our ad hoc
174 mixed precision inner product FMA defined in Assumption 2.3 is a level-2 BLAS operation to work
175 on any two different precision types. Although our analysis concerns accuracy and stability and
176 leaves out timing results of various hardwares, we add a general timing statement to Assumption 2.3
177 that is analogous to that of TensorCore: the mixed precision FMA inner product performs at least
178 2 times faster than the inner product in the higher precision. Note that the TensorCore FMA
179 block performs matrix-matrix multiply and accumulate up to 8 times faster than fp32, and up to 16
180 times faster than fp64 (see), and our ad hoc timing assumption is in conservative in comparison.
181 Nonetheless, this gives a vague insight into the trade-offs between speediness and accuracy from
182 some mixed precision computations. The full precision multiplication in Assumption 2.3 is exact
183 when the low precision type is fp16 and the high precision type of fp32 due to their precisions
184 and exponent ranges. As a quick proof, consider $x^{(\mathrm{fp16})} = \pm\mu_x 2^{\eta_x - 11}, y^{(\mathrm{fp16})} = \pm\mu_y 2^{\eta_y - 11}$ where
185 $\mu_x, \mu_y \in [0, 2^{11} - 1]$ and $\eta_x, \eta_y \in [-15, 16]$, and note that the significand and exponent ranges for
186 fp32 are $[0, 2^{24} - 1]$ and $[-127, 128]$. Then the product in full precision is

187
$$x^{(\mathrm{fp16})} y^{(\mathrm{fp16})} = \pm\mu_x \mu_y 2^{\eta_x + \eta_y + 2 - 24},$$

188 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

6

is exact. Thus, the summation and the final cast down operations are the only sources of rounding error in this inner product scheme.

ASSUMPTION 2.3. *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. Furthermore, we expect this procedure to be approximately twice as fast as if it were done entirely in the higher precision, and about the same as if it were done entirely in the lower precision.*

We now analyze the rounding error for the inner product scheme described in Assumption 2.3. Let $\mathbf{x}^{(l)}, \mathbf{y}^{(l)}$ be m-length vectors stored in some low precision float, $\mathbb{F}_l$, s_k be the exact k^{th} partial sum, and $\hat{s_k}$ be s_k computed with FLOPs. Then,

$$\hat{s_1} = \mathrm{fl}(\mathbf{x}[1]\mathbf{y}[1]) = \mathbf{x}[1]\mathbf{y}[1],$$

$$\hat{s_2} = \mathrm{fl}(\hat{s_1} + \mathbf{x}[2]\mathbf{y}[2]) = (\mathbf{x}[1]\mathbf{y}[1] + \mathbf{x}[2]\mathbf{y}[2])(1 + \delta_1^{(h)}),$$

$$\hat{s_3} = \mathrm{fl}(\hat{s_2} + \mathbf{x}[3]\mathbf{y}[3]) = \left[(\mathbf{x}[1]\mathbf{y}[1] + \mathbf{x}[2]\mathbf{y}[2])(1 + \delta_1^{(h)}) + \mathbf{x}[3]\mathbf{y}[3]\right](1 + \delta_2^{(h)}).$$

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

$$(2.9) \qquad \hat{s_m} = (\mathbf{x}[1]\mathbf{y}[1] + \mathbf{x}[2]\mathbf{y}[2])\prod_{k=1}^{m-1}(1 + \delta_k^{(h)}) + \sum_{i=3}^{n}\mathbf{x}[i]\mathbf{y}[i]\left(\prod_{k=i-1}^{m-1}(1 + \delta_k^{(h)})\right).$$

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

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

Suppose that $|\mathrm{fl}(\mathbf{x}^\top\mathbf{y})|$ is smaller than the largest representable number in the lower precision. Casting this down to $\mathbb{F}_l$ results in the forward errors,

$$(2.11) \qquad \mathrm{fl}(\mathbf{x}^\top\mathbf{y}) = (\mathbf{x} + \tilde{\Delta}\mathbf{x})^\top\mathbf{y} = \mathbf{x}^\top(\mathbf{y} + \tilde{\Delta}\mathbf{y}),$$

where $|\tilde{\Delta}\mathbf{x}| \le ((1 + u^{(l)})(1 + \gamma_{m-1}^{(h)}) - 1)|\mathbf{x}|$ and $|\tilde{\Delta}\mathbf{y}| \le ((1 + u^{(l)})(1 + \gamma_{m-1}^{(h)}) - 1)|\mathbf{y}|$.

Without any analysis, we expect that a mixed precision inner product described in Assumption 2.3 should perform better than if it were computed entirely in the lower precision and worse than if it were computed entirely in the high precision. This hypothesis is proven correct since,

$$\gamma_m^{(l)} > ((1 + u^{(l)})(1 + \gamma_{m-1}^{(h)}) - 1) > \gamma_m^{(h)},$$

where the lower and upper bounds are derived from the uniform precision error bound from (2.7). Our analysis in (2.11) shows us that the most of the errors are from the higher precision summation, $\gamma_{m-1}^{(h)}$, and the cast down operation adds $u^{(l)}$. The impact of the cast down step is measured relative to the length of the vector, m, and the disparity in the two precisions, $M_{l,h} := u^{(l)}/u^{(h)}$, since these two factors determine which one out of $u^{(l)}$ and $mu^{(h)}$ is the leading order term. There are 3 cases to consider.

Case 1: ($m \ll M_{l,h}$) The leading order term is $u^{(l)}$ and the mixed precision inner product can claim its superiority in accuracy only in comparison to the inner product computed in the lower

7

precision. Therefore, this inner product mixed precision successfully reduces the error from $mu^{(l)}$) to $u^{(l)}$ with no apparent improvements in speed.

Case 2: $(m = M_{l,h})$ Both terms are now leading order. Thus, this is still an improvement in comparison to the lower precision arithmetic as the error is reduced from $mu^{(l)}$ to $2u^{(l)}$. Comparing this to the inner product computed entirely in the higher precision shows that the error has doubled from $mu^{(h)}$ to $2mu^{(h)}$, but gained a factor of 2 speed-up in timing instead. One can argue that the loss in accuracy and the improvement in speed have essentially canceled each other out, but this can be reevaluated if the speed-up greatly exceeds a factor of 2.

Case 3: $(m \gg M_{l,h})$ Now the second term $\gamma_{m-1}^{(h)}$ is the leading order term. As in the above two cases, this is an improvement in the context of the low precision accuracy since the error has been reduced from $\gamma_m^{(l)}$ to $\gamma_{m/M_{l,h}}^{(l)} \equiv \gamma_m^{(h)}$. Since $u^{(l)} = M_{l,h}u^{(h)} \ll mu^{(h)}$, the error from the mixed precision inner product is in the same *order* as the error from carrying the computation out in the higher precision. Therefore, we can expect about the same level of accuracy but a factor of 2 or greater reduction in speed when compared to the higher precision.

While the analysis in the above cases establish 3 regimes of trade-offs between accuracy and speed in mixed precision computing, the remainder of this paper focuses only on accuracy and does not consider the impact of mixed precision computations on speed. Readers should refer to timing studies such as ..... Finally, we present alternate ways of understanding the error bound in (2.11). This bound can be simplified using the following rules,

$$(1 + u^{(l)})(1 + \gamma_{m-1}^{(h)}) - 1 \le \gamma_{M_{l,h}+m-1}^{(h)} = \gamma_{1+(m-1)/M_{l,h}}^{(l)}, \quad M_{l,h} = u^{(l)}/u^{(h)},$$

$$(1 + u^{(l)})(1 + \gamma_{m-1}^{(h)}) - 1 \le u^{(l)} + \gamma_{m-1}^{(h)} + \min\{u^{(l)}, \gamma_{m-1}^{(h)}\}, \quad \gamma_{m-1}^{(h)} < 1.$$

These two alternate bounds can be useful in different contexts. Nevertheless, they both indicate that the error is $\mathcal{O}(u^{(l)} + mu^{(h)} + mu^{(l)}u^{(h)})$ and are slightly larger than the original bound, on the LHS. We summarize these ways of combining γ terms of different precisions in Lemma 2.4, which is a simple modification of some of the rules from Lemma 2.2.

LEMMA 2.4. *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 $1 \gg u_l \gg u_h > 0$, and k_l, k_h small enough such that $\max\{\gamma_{k_h}^{(h)}, \gamma_{k_l}^{(l)}\} < 1/2$. Then the following rules help us accumulate γ's of different precisions,*

$$(2.12) \qquad\qquad\qquad\qquad \gamma_{k_h}^{(h)}\gamma_{k_l}^{(l)} \le \min\{\gamma_{k_h}^{(h)}, \gamma_{k_l}^{(l)}\},$$

$$(2.13) \qquad\qquad\qquad (1 + \tilde{\gamma}_{k_l}^{(l)})(1 + \tilde{\gamma}_{k_h}^{(h)}) - 1 = \tilde{\gamma}_{k_l}^{(l)} + \tilde{\gamma}_{k_h}^{(h)}.$$

Note that (2.13) drops the term $\tilde{\gamma}_{k_l}^{(l)}\tilde{\gamma}_{k_h}^{(h)}$ since both $\tilde{\gamma}_{k_l}^{(l)}$ and $\tilde{\gamma}_{k_h}^{(h)}$ are larger than their product and this product can be swept under the small integer $c > 0$ assumption implicitly included in the $\tilde{\gamma}$ notation.

Equations (2.10) and (2.11) are crucial for our analysis in section 4 since they closely resemble the TensorCore FMA block which can return 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 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 instead after every matrix multiplication

8

and still take advantage of the better storage properties of lower precision types. In general, 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).

We have demonstrated a need for rounding error analysis that is accurate for mixed precision procedures and analyzed the inner product in a mixed precision procedure similar to that of TensorCore. We will use this to analyze some QR factorization algorithms. In section 3, we introduce various Householder QR algorithms and the general framework for the standard rounding error analysis for these algorithms which 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 [15]). 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, $\mathbf{P_v}$, such that $\mathbf{P_v}$ zeros out $\mathbf{x}$ below the first element.*

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

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

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 $i = 1, 2, \cdots, n$,
Step 1) Compute $\mathbf{v}$ and β that zeros out the ith column of $\mathbf{A}$ beneath a_{ii} (see alg. 2), and
Step 2) Apply $\mathbf{P_v}$ 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 [12]. Let $\mathbf{P}_i$ represent the ith Householder transformation of this algorithm.

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

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

9

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

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

Algorithm 2: β, $\mathbf{v}$, $\sigma = \mathtt{hh\_vec}(\mathbf{x})$. Given a vector $\mathbf{x} \in \mathbb{R}^n$, return $\mathbf{v}$, β, σ that satisfy $(I - \beta\mathbf{v}\mathbf{v}^{\top})\mathbf{x} = \sigma\hat{e}_1$ 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 $(I - \beta\mathbf{v}\mathbf{v}^{\top})\mathbf{x} = \pm\|\mathbf{x}\|_2\hat{e}_1 = \sigma\hat{e}_1$

1 $\mathbf{v} \leftarrow \mathtt{copy}(\mathbf{x})$
2 $\sigma \leftarrow -\mathrm{sign}(\mathbf{x}[1])\|\mathbf{x}\|_2$
3 $\mathbf{v}[1] \leftarrow \mathbf{x}[1] - \sigma$
4 $\beta \leftarrow -\frac{\mathbf{v}[1]}{\sigma}$
5 **return** β, $\mathbf{v}/\mathbf{v}[1]$, σ

Algorithm 3: $\mathbf{V}$, $\boldsymbol{\beta}$, $\mathbf{R} = \mathtt{HQR2}(A)$. 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 $\boldsymbol{\beta} \in \mathbb{R}^n$, and upper triangular matrix $\mathbf{R}$. An orthogonal matrix $\mathbf{Q}$ can be generated from $\mathbf{V}$ and $\boldsymbol{\beta}$, and $\mathbf{QR} = \mathbf{A}$.

Input: $A \in \mathbb{R}^{m \times n}$ where $m \geq n$.
Output: $\mathbf{V}$, $\boldsymbol{\beta}$, $\mathbf{R}$

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

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 ith Householder vector and constant. In alg. 3, the we compute the Householder vector and constant by using alg. 2 to $\mathbf{A}[i : m, i]$. Let us consider zeroing out any vector $\mathbf{x} \in \mathbb{R}^m$ below its first component with a Householder transformation. We first calculate σ as is implemented in line 2 of alg. 2.

(3.3) $$\mathrm{fl}(\sigma) = \hat{\sigma} = \mathrm{fl}(-\mathrm{sign}(\mathbf{x}[1])\|\mathbf{x}\|_2) = \sigma + \Delta\sigma, \quad |\Delta\sigma| \leq \gamma_{\mathrm{m}+1}|\sigma|.$$

Note that the backward error incurred here accounts for an inner product of a vector in $\mathbb{R}^m$ with itself and a square root operation to get the 2-norm. Let $\tilde{\mathbf{v}}[1] \equiv \mathbf{x}[i] - \sigma$, the penultimate value $\mathbf{v}[1]$. The subtraction adds a single additional rounding error via

(3.4) $$\mathrm{fl}(\tilde{\mathbf{v}}[1]) = \tilde{\mathbf{v}}[1] + \Delta\tilde{\mathbf{v}}[1] = (1 + \delta)(\mathbf{x}[i] - \sigma - \Delta\sigma) = (1 + \theta_{m+2})\tilde{\mathbf{v}}[1]$$

where the last equality is granted because the sign of σ is chosen to prevent cancellation. Since alg. 2 normalizes the Householder vector so that its first component is 1, the remaining components

10

319 of $\mathbf{v}$ are divided by $\mathrm{fl}(\tilde{\mathbf{v}}_1)$ incurring another single rounding error. As a result, the components of
320 $\mathbf{v}$ computed with FLOPs have error $\mathrm{fl}(\mathbf{v}[j]) = \mathbf{v}[j] + \Delta\mathbf{v}[j]$ where

321 (3.5)
$$|\Delta\mathbf{v}[j]| \leq \begin{cases} 0, & j = 1 \\ \gamma_{1+2(m+2)}|\mathbf{v}[j]| = \tilde{\gamma}_m|\mathbf{v}[j]|, & j = 2 : m - i + 1. \end{cases}$$

322 Since $1 + 2(m + 2) + = \mathcal{O}(m)$, we have swept that minor difference between under our use of the $\tilde{\gamma}$
323 notation defined in Lemma 2.1. Next, we consider the Householder constant, β, as is computed in
324 line 4 of alg. 2.

325 (3.6)
$$\hat{\beta} = \mathrm{fl}\left(-\tilde{\mathbf{v}}[1]/\hat{\sigma}\right) = -(1 + \delta)\frac{\tilde{\mathbf{v}}[1] + \Delta\tilde{\mathbf{v}}[1]}{\sigma + \Delta\sigma}$$

326 (3.7)
$$= \frac{(1 + \delta)(1 + \theta_{m+2})}{(1 + \theta_{m+1})}\beta = (1 + \theta_{3m+5})\beta$$

327 (3.8)
328
$$= \beta + \Delta\beta, \text{ where } |\Delta\beta| \leq \tilde{\gamma}_m\beta.$$

329 We have shown (3.6) to keep our analysis simple in section 4 and (3.7) and (3.8) show that the
330 error incurred from calculating of $\|\mathbf{x}\|_2$ accounts for the vast majority of the rounding error so far.
331 At iteration i, we replace $\mathbf{x}$ with $\mathbf{A}[i : m, i] \in \mathbb{R}^{m-i+1}$ and the ith Householder constant and vector
332 $(\hat{\beta}_i, \mathbf{v}_i)$ both have errors bounded by $\tilde{\gamma}_{m-i+1}$.
333   *Applying a Single Householder Transformation.* Now we consider lines 4-6 of alg. 3. At iteration
334 i, we set $\mathbf{A}[i + 1 : m]$ to zero and replace $\mathbf{A}[i, i]$ with σ computed from alg. 2. Therefore, we now
335 need to calculate the errors for applying a Householder transformation to the remaining columns,
336 $\mathbf{A}[i : m, i + 1 : n]$ with the computed Householder vector and constant. This is the most crucial
337 building block of the rounding error analysis for any variant of HQR because the $\mathbf{R}$ factor is formed
338 by applying the Householder transformations to $\mathbf{A}$ and the $\mathbf{Q}$ factor is formed by applying them
339 in reverse order to the identity. Both of the blocked versions in subsection 3.2 and subsection 3.3
340 also require efficient implementations of this step, although they may be implemented slightly
341 differently. For example, BQR in alg. 5 uses level-3 BLAS operations to apply multiple Householder
342 transformations at once whereas the variant of HQR in alg. 3 can only use level-2 BLAS operations
343 to apply Householder transformations.
344   A Householder transformation is applied through a series of inner and outer products, since
345 Householder matrices are rank-1 updates of the identity. That is, computing $\mathbf{P}_\mathbf{v}\mathbf{x}$ for any $\mathbf{x} \in \mathbb{R}^m$
346 is as simple as computing

347 (3.9)
$$\mathbf{y} := \mathbf{P}_\mathbf{v}\mathbf{x} = \mathbf{x} - (\beta\mathbf{v}^\top\mathbf{x})\mathbf{v}.$$

348 Let us assume that $\mathbf{x}$ is an exact vector and there were errors incurred in forming $\mathbf{v}$ and β. The
349 errors incurred from computing $\mathbf{v}$ and β need to be included in addition to the new rounding errors
350 accumulating from the action of applying $\mathbf{P}_\mathbf{v}$ to a column. In practice, $\mathbf{x}$ would be a column in
351 $\mathbf{A}^{(i-1)}[i + 1 : m, i + 1 : n]$, where the superscript $(i - 1)$ indicates that this submatrix of $\mathbf{A}$ has
352 already been transformed by $i - 1$ Householder transformations that zeroed out components below
353 $\mathbf{A}_{j,j}$ for $j = 1 : i - 1$. We show the error for forming $\mathrm{fl}\left(\hat{\mathbf{v}}^\top\mathbf{x}\right)$ where we let $\mathbf{v}, \mathbf{x} \in \mathbb{R}^m$:

354
$$\mathrm{fl}\left(\hat{\mathbf{v}}^\top\mathbf{x}\right) = (1 + \theta_m)(\mathbf{v} + \Delta\mathbf{v})^\top\mathbf{x}.$$

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

356
$$\hat{\mathbf{w}} = (1 + \theta_m)(1 + \delta)(1 + \tilde{\delta})(\beta + \Delta\beta)(\mathbf{v} + \Delta\mathbf{v})^\top\mathbf{x}(\mathbf{v} + \Delta\mathbf{v}),$$

11

357 where θ_m is from computing the inner product $\hat{\mathbf{v}}^\top \mathbf{x}$, and δ and $\tilde{\delta}$ are from multiplying β, $\mathrm{fl}(\hat{\mathbf{v}}^\top \mathbf{x})$,
358 and $\hat{\mathbf{v}}$ together. We can write

$$\hat{\mathbf{w}} = \mathbf{w} + \Delta\mathbf{w}, \;\; |\Delta\mathbf{w}| \leq \tilde{\gamma}_m |\beta| |\mathbf{v}|^\top |\mathbf{x}| |\mathbf{v}|.$$

360 Finally, we can add in the vector subtraction operation and complete the rounding error analysis
361 of applying a Householder transformation to any vector:

362 (3.10) $\qquad \mathrm{fl}(\hat{\mathbf{P}}_{\mathbf{v}}\mathbf{x}) = \mathrm{fl}(\mathbf{x} - \hat{\mathbf{w}}) = (1+\delta)(\mathbf{x} - \mathbf{w} - \Delta\mathbf{w}) = \mathbf{y} + \Delta\mathbf{y} = (\mathbf{P}_{\mathbf{v}} + \Delta\mathbf{P}_{\mathbf{v}})\mathbf{x},$

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

364 (3.11) $$\|\Delta\mathbf{y}\|_2 \leq \tilde{\gamma}_m \|\mathbf{x}\|_2.$$

365 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
366 its Frobenius norm by using $\Delta\mathbf{P}_{\mathbf{v}}[i,j] = \frac{1}{\|\mathbf{x}\|_2^2}\Delta\mathbf{y}[i]\mathbf{x}[j]$,

367 (3.12) $$\|\Delta\mathbf{P}_{\mathbf{v}}\|_F = \left(\sum_{i=1}^m \sum_{j=1}^m \left(\frac{1}{\|\mathbf{x}\|_2^2} \Delta\mathbf{y}[i]\mathbf{x}[j] \right)^2 \right)^{1/2} = \frac{\|\Delta\mathbf{y}\|_2}{\|\mathbf{x}\|_2} \leq \tilde{\gamma}_m,$$

368 where the last inequality is a direct application of (3.11).
369 　　*Applying many successive Householder transformations.* Consider applying a sequence of trans-
370 formations 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 transforma-
371 tions 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
372 $\mathbf{R} = \mathbf{Q}^\top \mathbf{A} = \mathbf{P}_n \cdots \mathbf{P}_1 \mathbf{A}$. Lemma 3.2 is very useful for any sequence of transformations, where
373 each transformation has a known bound. We will invoke this lemma to prove Lemma 3.3, and use
374 it in future sections for other sequential transformations.

　　LEMMA 3.2. *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*

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

375 　　LEMMA 3.3. *Consider applying a sequence of transformations $\mathbf{Q} = \mathbf{P}_r \cdots \mathbf{P}_2 \mathbf{P}_1$ onto vector*
376 $\mathbf{x} \in \mathbb{R}^m$ *to form $\hat{\mathbf{y}} = \mathrm{fl}(\hat{\mathbf{P}}_r \cdots \hat{\mathbf{P}}_2 \hat{\mathbf{P}}_1 \mathbf{x})$, where $\hat{\mathbf{P}}_k$'s are Householder transformations constructed*
377 *from $\hat{\beta}_k$ and $\hat{\mathbf{v}}_k$. These Householder vectors and constants are computed via alg. 2 and the rounding*
378 *errors are bounded by (3.5) and (3.8). If each transformation is computed via (3.9), then*

379 (3.13) $$\hat{\mathbf{y}} = \mathbf{Q}(\mathbf{x} + \Delta\mathbf{x}) = (\mathbf{Q} + \Delta\mathbf{Q})\mathbf{x} = \hat{\mathbf{Q}}\mathbf{x},$$

380 (3.14) $$\|\Delta\mathbf{y}\|_2 \leq r\tilde{\gamma}_m \|\mathbf{x}\|_2, \;\; \|\Delta\mathbf{Q}\|_F \leq r\tilde{\gamma}_m.$$

382 　　*Proof.* Applying Lemma 3.2 directly to $\mathbf{Q}$ yields

383 $$\|\Delta\mathbf{Q}\|_F = \left\| \prod_{j=1}^r (\mathbf{P}_j + \Delta\mathbf{P}_j) - \prod_{j=1}^r \mathbf{P}_j \right\|_F \leq \left(-1 + \prod_{j-1}^r (1+\tilde{\gamma}_{m-j+1})^r \right) \prod_{j=1}^n \|\mathbf{P}_j\|_2$$

384 $$\leq -1 + (1 + \tilde{\gamma}_m)^r,$$

386 since $\mathbf{P}_j$'s are orthogonal and have 2-norm, 1, and $m - j + 1 \leq m$. While we omit the details here,
387 we can show that $(1 + \tilde{\gamma}_m)^r - 1 \leq r\tilde{\gamma}_m$ using the argument from Lemma 2.1 if $r\tilde{\gamma}_m \leq 1/2$. □

In this error analysis, the prevailing bound for errors at various stages of forming and applying a Householder transformation is $\tilde{\gamma}_m$ where m corresponds to the dimension of the transformed vectors. In Lemma 3.3, a factor of r is introduced for applying r Householder transformations to form the term $r\tilde{\gamma}_m \approx rmu$. Therefore, we can expect that the columnwise norm error for a thin QR factorization should be $\mathcal{O}(mnu)$ for a full rank matrix. In Theorem 3.4, we formalize this by applying Lemma 3.3 directly and also show the result of converting these columnwise bounds to matrix norm bounds.

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

We gather these results into Theorem 3.4.

THEOREM 3.4. *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. Then,*

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

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

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

$$\|\hat{\mathbf{Q}}\hat{\mathbf{R}} - \mathbf{A}\|_F \leq n^{3/2}\tilde{\gamma}_m\|\mathbf{A}\|_F.$$

Note that the last backward error result follows from the columnwise forward errors for $\hat{\mathbf{R}}$ and $\hat{\mathbf{Q}}$. Out of all of these different ways of measuring the error from computing a QR factorization (forward/backward errors for column/matrix norms), we will focus on $\|\hat{\mathbf{Q}} - \mathbf{Q}\|_F$, a measure of orthogonality of the $\mathbf{Q}$ factor for the remainder of section 3 and for section 4. In section 5, we will turn to the backward norm error, $\|\hat{\mathbf{Q}}\hat{\mathbf{R}} - \mathbf{A}\|_F$ since it can actually be computed.

The content of this section shows the standard rounding error analysis in [12] where some important stages are summarized in (3.5), (3.8), and (3.14), which we will modify to different mixed precision settings in section 4. 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 section relies on the WY representation described in [4] instead of the storage-efficient version of [19], even though both are known to be just as numerically stable as HQR.

3.2.1. The WY Representation. A convenient matrix representation that accumulates r Householder reflectors is known as the WY representation (see [4, 9]). Lemma 3.5 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. This algorithm assumes that the Householder vectors, $\mathbf{V}$, and constants,$\boldsymbol{\beta}$, have already been computed. Since the $\mathbf{Y}$ factor is exactly $\mathbf{V}$, we only need to compute the $\mathbf{W}$ factor.

13

428   LEMMA 3.5. *Suppose* $\mathbf{X}^{(j)} = \mathbf{I} - \mathbf{W}^{(j)}\mathbf{Y}^{(j)\top} \in \mathbb{R}^{m \times m}$ *is an orthogonal matrix with* $\mathbf{W}^{(j)}, \mathbf{Y}^{(j)} \in$
429 $\mathbb{R}^{m \times j}$. *Let us define* $\mathbf{P} = \mathbf{I} - \beta\mathbf{v}\mathbf{v}^\top$ *for some* $\mathbf{v} \in \mathbb{R}^m$ *and let* $\mathbf{z}^{(j+1)} = \beta\mathbf{X}^{(j)}\mathbf{v}$. *Then,*

430
$$\mathbf{X}^{(j+1)} = \mathbf{X}^{(j)}\mathbf{P} = \mathbf{I} - \mathbf{W}^{(j+1)}\mathbf{Y}^{(j+1)\top},$$

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

    Input: $\mathbf{V} \in \mathbb{R}^{m \times r}$, $\boldsymbol{\beta} \in \mathbb{R}^r$ where $m > r$.
    Output: $\mathbf{W}$
1 Initialize: $\mathbf{W} := \boldsymbol{\beta}_1\mathbf{V}[:,1]$.   `/* Y is V. */`
2 **for** $j = 2 : r$ **do**
3      $\mathbf{z} \leftarrow \boldsymbol{\beta}_j\left[\mathbf{V}[:,j] - \mathbf{W}\left(\mathbf{V}[:,1:j-1]^\top\mathbf{V}[:,j]\right)\right]$
4      $\mathbf{W} \leftarrow [\mathbf{W}\quad\mathbf{z}]$ `/* Update `$\mathbf{W}$` to an `m`-by-`j` matrix. */`
5 **return** $\mathbf{W}$

---

432   In HQR, $\mathbf{A}$ is transformed into an upper triangular matrix $\mathbf{R}$ by identifying a Householder
433 transformation that zeros out a column below the diagonal, then applying that Householder trans-
434 formation to the bottom right partition. For example, the kth Householder transformation finds
435 an $m - k + 1$ sized Householder transformation that zeros out column k below the diagonal and
436 then applies it to the $(m - k + 1)$-by-$(n - k)$ partition of the matrix, $\mathbf{A}[k : m, k + 1 : n]$. Since
437 the $k + 1^{st}$ column is transformed by the kth Householder transformation, this algorithm must be
438 executed serially as shown in alg. 3. The highest computational burden at each iteration falls on
439 alg. 3 line 6, which requires Level-2 BLAS operations when computed efficiently.
440   In contrast, BQR replaces this step with Level-3 BLAS operations by partitioning $\mathbf{A}$ into blocks
441 of columns. Let $\mathbf{A} = [\mathbf{C}_1 \cdots \mathbf{C}_N]$ where $\mathbf{C}_1, \cdots, \mathbf{C}_{N-1}$ are each m-by-r, and $\mathbf{C}_N$ holds the remaining
442 columns. The kth block, $\mathbf{C}_k$, is transformed with HQR (alg. 3), and the WY representation of these
443 r successive Householder transformations is constructed as in alg. 4. We write the WY update as

444 (3.15)
$$\mathbf{X}_k = \mathbf{I}_m - \mathbf{W}_k\mathbf{Y}_k^\top = \mathbf{P}_k^{(1)} \cdots \mathbf{P}_k^{(r)}.$$

445 Thus far, algs. 3 and 4 are rich in Level-2 BLAS operations. Next, $\mathbf{I} - \mathbf{Y}_k\mathbf{W}_k^\top$ is applied to
446 $[\mathbf{C}_2 \cdots \mathbf{C}_N]$ with two Level-3 BLAS operations as shown in line 5 of alg. 5. BQR performs ap-
447 proximately $1 - \mathcal{O}(1/N)$ fraction of its FLOPs in Level-3 BLAS operations (see section 5.2.3 of
448 [9]), and can reap the benefits from the accelerated block FMA feature of TensorCore. Note that
449 BQR does require strictly more FLOPs when compared to HQR, but these additional FLOPs are
450 negligble in standard precision and does not impact the numerical stability. A pseudoalgorithm for
451 BQR is shown in alg. 5 where we assume that $n = Nr$ to make our error analysis in section 3.2.2
452 simple. In practice, an efficient implementation might require r to be a power of two or a product
453 of small prime factors and result a thinner N^{th} block compared to the rest. This discrepancy is
454 easily fixed by padding the matrix with zeros, a standard procedure for standard algorithms like
455 the Fast Fourier Transform (FFT). For any variable $x \in \{\mathbf{X}, \mathbf{W}, \mathbf{Y}, \mathbf{z}, \beta, \mathbf{v}, \mathbf{P}\}$, $x_k^{(j)}$ corresponds to
456 the jth update for the kth block.

14

Algorithm 5: $\mathbf{Q}, \mathbf{R} \leftarrow \texttt{blockHQR}(\mathbf{A}, r)$: 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 $N = \frac{n}{r}$
    // 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 $\mathbf{V}_i, \boldsymbol{\beta}_i, \mathbf{C}_i \leftarrow \texttt{hhQR}(\mathbf{C}_i)$ `/* Algorithm 3 */`
4 $\mathbf{W}_i \leftarrow \texttt{buildWY}(\mathbf{V}_i, \boldsymbol{\beta}_i)$ `/* Algorithm 4 */`
5 $[\mathbf{C}_{i+1} \cdots \mathbf{C}_N] \mathrel{-}= \mathbf{V}_i \left(\mathbf{W}_i^\top [\mathbf{C}_{i+1} \cdots \mathbf{C}_N] \right)$ `/* 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 $\mathbf{Q}[(i-1)r+1 : m, (i-1)r+1 : n] \mathrel{-}= \mathbf{W}_i \left(\mathbf{V}_i^\top \mathbf{Q}[(i-1)r+1 : m, (i-1)r+1 : n] \right)$
9 **return** $\mathbf{Q}, \mathbf{A}$

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 W factor, and 3) updating the remaining blocks with the WY representation. We have adapted the analysis from [12] to fit this exact variant, and denote $\hat{\mathbf{Q}}_{BQR}, \hat{\mathbf{R}}_{BQR}$ to be the outputs from alg. 5. First, we analyze the error accumulated from updating $\mathbf{X}_k^{(j-1)}$ to $\mathbf{X}_k^{(j)}$, which applies a rank-1 update via the subtraction of the outer product $\hat{\mathbf{z}}_k^{(j)} \hat{\mathbf{v}}_k^{(j)\top}$. Since $\mathbf{z}_k^{(j)} = \beta_k^{(j)} \mathbf{X}_k^{(j-1)} \mathbf{v}_k^{(j)}$, this update requires a single Householder transformation on the right side in the same efficient implementation that is discussed in (3.9),

$$(3.16) \qquad \hat{\mathbf{X}_k^{(j)}} = \hat{\mathbf{X}}_k^{(j-1)} - \text{fl}(\hat{\beta}_k^{(j-1)} \hat{\mathbf{X}}_k^{(j-1)} \hat{\mathbf{v}}_k^{(j-1)}) \hat{\mathbf{v}}_k^{(j)\top} = \hat{\mathbf{X}}_k^{(j-1)} (\mathbf{P}_k^{(j)} + \Delta \mathbf{P}_k^{(j)}),$$

where $\|\Delta \mathbf{P}_k^{(j)}\|_F \leq \tilde{\gamma}_{m-(k-1)r}$. Since $\hat{\mathbf{X}}_k^{(1)} = \mathbf{I} - \hat{\beta}_k^{(1)} \hat{\mathbf{v}}_k^{(1)} \hat{\mathbf{v}}_k^{(1)\top} = \mathbf{P}_k^{(1)} + \Delta \mathbf{P}_k^{(1)}$, we can travel up the recursion relation in (3.16) and use Lemma 3.2 to find

$$(3.17) \qquad \|\Delta \mathbf{X}_k^{(j)}\|_F \leq j \tilde{\gamma}_{m-(k-1)r}.$$

HQR within each block: line 3 of alg. 5. We apply Algorithm 3 to the kth block, $\hat{\mathbf{X}}_{k-1} \cdots \hat{\mathbf{X}}_1 \mathbf{C}_k$, which applies r more Householder transformations to columns that had been transformed by $(k-1)$ WY transformations in prior iterations. The upper trapezoidal factor that results from applying HQR to $\mathbf{C}_k^{((k-1)r)}$ corresponds to the $(k-1)r + 1^{st}$ to kr^{th} columns of $\hat{\mathbf{R}}_{BQR}$, and applying Lemmas 3.2 and 3.3 yields

$$\|\hat{\mathbf{R}}_{BQR}[:, j] - \mathbf{R}[:, j]\|_2 \leq r \tilde{\gamma}_m \|\hat{\mathbf{X}}_{k-1} \cdots \hat{\mathbf{X}}_1^\top \mathbf{C}_k[:, j]\|_2, \quad j = (k-1)r + 1 : kr.$$

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. Since the columns of $\hat{\mathbf{Y}}_k$ are simply $\{\hat{\mathbf{v}}_k^{(}j)\}$ built in alg. 3 the errors for forming these are

15

shown in (3.5) where m should be replaced by $m - (k-1)r$. The Householder constants, $\hat{\beta}_k^{(j)}$ are bounded by (3.8) modified similarly. Thus, $\mathbf{z}_k^{(j)}$ is the only newly computed quantity. Using (3.5), (3.8), and (3.17), we find

$$\|\Delta \mathbf{z}_k^{(j)}\|_2 = \|\Delta \mathbf{X}_k^{(j-1)} \hat{\beta}_k^{(j)} \hat{\mathbf{v}}_k^{(j)}\|_2 \le \|\Delta \mathbf{X}_k^{(j)}\|_2 \|\hat{\beta}_k^{(j)} \hat{\mathbf{v}}_k^{(j)}\|_2$$

$$\le \|\Delta \mathbf{X}_k^{(j)-1}\|_F \|\hat{\beta}_k^{(j)} \hat{\mathbf{v}}_k^{(j)}\|_2$$

$$\le \left((1 + (j-1)\tilde{\gamma}_{m-(k-1)r})(1 + \tilde{\gamma}_{m-(k-1)r}) - 1 \right) \|\beta_k^{(j)} \mathbf{v}_k^{(j)}\|_2$$

$$\le j\tilde{\gamma}_{m-(k-1)r} \|\mathbf{z}_k^{(j)}\|_2$$

Componentwise bounds follow immediately, and are summarized in Lemma 3.6.

LEMMA 3.6. *Consider the construction of the WY representation for the kth partition of matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ given a set of Householder constants and vectors, $\{\beta_k^{(j)}\}_{j=1}^r$ and $\{\mathbf{v}_k^{(j)}\}$ via alg. 4. Then,*

(3.18)
$$\hat{\mathbf{z}}_k^{(j)} = \mathbf{z}_k^{(j)} + \Delta \mathbf{z}_k^{(j)}, \quad |\Delta \mathbf{z}_k^{(j)}| \le j\tilde{\gamma}_{m-(k-1)r} |\mathbf{z}_k^{(j)}|$$

(3.19)
$$\hat{\mathbf{v}}_k^{(j)} = \mathbf{v}_k^{(j)} + \Delta \mathbf{v}_k^{(j)}, \quad |\Delta \mathbf{v}_k^{(j)}| \le \tilde{\gamma}_{m-(k-1)r} |\mathbf{v}_k^{(j)}|,$$

where the second bound is derived from (3.5).

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 5 of alg. 5. We now consider applying $\mathbf{X}_k := \mathbf{I} - \mathbf{W}_k \mathbf{Y}_k^\top$ to some matrix, $\mathbf{B}$. In practice, $\mathbf{B}$ is the bottom right submatrix, $[\mathbf{C}_{k+1} \cdots \mathbf{C}_N][(k-1)r + 1 : m, :]$. We can apply (3.17) directly to the columns of $\mathbf{B}$,

(3.20)
$$\|\mathrm{fl}(\hat{\mathbf{X}}_k \mathbf{B}[:, j])\|_2 = \|\mathrm{fl}(\hat{\mathbf{X}}_k^{(r)} \mathbf{B}[:, j])\|_2 \le r\tilde{\gamma}_{m-(k-1)r} \|\mathbf{B}[:, j]\|_2$$

A normwise bound for employing 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 3.2 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 3.3. 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 $\mathbf{R}_{BQR}$, and apply the transpose to $\hat{e}_i$'s to form the bounds for $\mathbf{Q}_{BQR}$. Then,

(3.21)
$$\left\| \prod_{k=1}^N (\mathbf{X}_k + \Delta \mathbf{X}_k) - \prod_{k=1}^N \mathbf{X}_k \right\|_F \le \left(-1 + \sum_{k=1}^N (1 + r\tilde{\gamma}_{m-(k-1)r}) \right) \le rN\tilde{\gamma}_m \equiv n\tilde{\gamma}_m,$$

(3.22)
$$\|\hat{\mathbf{Q}}_{BQR} - \mathbf{Q}\|_F \le n^{3/2}\tilde{\gamma}_m.$$

We can also form the normwise bound for the j'^{th} column of $\hat{\mathbf{Q}}_{BQR}, \hat{\mathbf{R}}_{BQR}$. If we let $k' = \lceil j'/r \rceil^{th}$, then the j'^{th} column is the result of applying $k' - 1$ WY updates and an additional HQR. Applying Lemma 3.2 yields

(3.23)
$$\|\Delta \mathbf{R}_{BQR}[:, j']\|_2 \le rk'\tilde{\gamma}_m \|\mathbf{A}[:, j]\|_2$$

(3.24)
$$\|\Delta \mathbf{Q}_{BQR}[:, j']\|_2 \le rk'\tilde{\gamma}_m$$

16

517 and near orthogonality of the **Q** factor is still achieved,

518 (3.25)
$$\|\Delta\mathbf{Q}_{BQR}\|_F = r\tilde{\gamma}_m \sum_{j=1}^{n} \lceil j/r \rceil = n^{3/2}\tilde{\gamma}_m.$$

519 The primary goal of the analysis presented in this section is to provide the basic skeleton for the
520 standard BQR rounding error analysis to make the generalization to mixed precision settings in
521 section 4 easier. Readers should refer to [9, 12] for full details.

522 **3.3. Block HQR with partitioned rows : Tall-and-Skinny QR (TSQR).** Some im-
523 portant problems that require QR factorizations of overdetermined systems include least squares
524 problems, eigenvalue problems, low rank approximations, as well as other matrix decompositions.
525 Although Tall-and-Skinny QR (TSQR) broadly refers to block QR factorization methods with row
526 partitions, we will discuss a specific variant of TSQR which is also known as the AllReduce algo-
527 rithm [18]. In this paper, the TSQR/AllReduce algorithm refers to the most parallel variant of
528 the block QR factorization algorithms discussed in [8]. A detailed description and rounding error
529 analysis of this algorithm can be found in [18], and we present a pseudocode for the algorithm in
530 alg. 6. Our initial interest in this algorithm came from its parallelizable nature, which is particu-
531 larly suitable to implementation on GPUs. Additionally, our numerical simulations (discussed in
532 section 5) show that TSQR can not only increase the speed but also outperform the traditional
533 HQR factorization in low precisions.

534 **3.3.1. TSQR/AllReduce Algorithm.** Algorithm 6 partitions the rows of a tall-and-skinny
535 matrix, **A**. HQR is performed on each of those blocks and pairs of **R** factors are combined to form
536 the next set of **A** matrices to be QR factorized. This process is repeated until only a single **R** factor
537 remains, and the **Q** factor is built from all of the Householder constants and vectors stored at each
538 level. The most gains from parallelization can be made in the initial level where the maximum
539 number of independent HQR factorizations occur. Although more than one configuration of this
540 algorithm may be available for a given tall-and-skinny matrix, the number of nodes available and
541 the shape of the matrix eliminate some of those choices. For example, a 1600-by-100 matrix can
542 be partitioned into 2, 4, 8, or 16 initial row-blocks but may be restricted by a machine with only
543 4 nodes, and a 1600-by-700 matrix can only be partitioned into 2 initial blocks. Our numerical
544 experiments show that the choice in the initial partition, which directly relates to the recursion
545 depth of TSQR, has an impact in the accuracy of the QR factorization.

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

553 *TSQR Notation.* We introduce new notation due to the multi-level nature of the TSQR algo-
554 rithm. In the final task of constructing **Q**, $\mathbf{Q}_j^{(i)}$ factors are aggregated from each block at each level.
555 Each $\mathbf{Q}_j^{(i)}$ factor from level i is partitioned such that two corresponding $\mathbf{Q}^{(i-1)}$ factors from level $i-1$
556 can be applied to them. The partition (approximately) splits $\mathbf{Q}_j^{(i)}$ into two halves, $[\tilde{\mathbf{Q}}_{j,1}^{(i)\top} \tilde{\mathbf{Q}}_{j,2}^{(i)\top}]^\top$.
557 The functions $\alpha(j)$ and $\phi(j)$ are defined such that $\mathbf{Q}_j^{(i)}$ is applied to the correct blocks from the level

17

below: $\tilde{\mathbf{Q}}^{(i+1)}_{\alpha(j),\phi(j)}$. For $j = 1, \cdots, 2^{L-i}$ 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.

Algorithm 6: $\mathbf{Q}, \mathbf{R} = \texttt{tsqr}(\mathbf{A}, L)$. 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 $\mathbf{Q}\mathbf{R} = \mathbf{A}$.

1 $h \leftarrow m2^{-L}$ // Number of rows.

   /* Split A into 2^L blocks. Note that level (i) has 2^{L-i} blocks.   */

2 **for** $j = 1 : 2^L$ **do**

3      $\mathbf{A}^{(0)}_j \leftarrow \mathbf{A}[(j-1)h + 1 : jh, :]$

   /* Store Householder vectors as columns of matrix $\mathbf{V}^{(i)}_j$, Householder

       constants as components of vector $\boldsymbol{\beta}^{(i)}_j$, and set up the next level.   */

4 **for** $i = 0 : L - 1$ **do**

      /* The inner loop can be parallelized.   */

5   **for** $j = 1 : 2^{L-i}$ **do**

6          $\mathbf{V}^{(i)}_{2j-1}, \boldsymbol{\beta}^{(i)}_{2j-1}, \mathbf{R}^{(i)}_{2j-1} \leftarrow \texttt{qr}(\mathbf{A}^{(i)}_{2j-1})$

7          $\mathbf{V}^{(i)}_{2j}, \boldsymbol{\beta}^{(i)}_{2j}, \mathbf{R}^{(i)}_{2j} \leftarrow \texttt{qr}(\mathbf{A}^{(i)}_{2j})$

8          $\mathbf{A}^{(i+1)}_j \leftarrow \begin{bmatrix} \mathbf{R}^{(i)}_{2j-1} \\ \mathbf{R}^{(i)}_{2j} \end{bmatrix}$

9 $\mathbf{V}^{(L)}_1, \boldsymbol{\beta}^{(L)}_1, \mathbf{R} \leftarrow \texttt{qr}(\mathbf{A}^{(L)}_1)$ // The final R factor is built.

10 $\mathbf{Q}^{(L)}_1 \leftarrow \texttt{hh\_mult}(\mathbf{V}^{(L)}_1, I_{2n \times n})$

   /* Compute $\mathbf{Q}^{(i)}$ factors by applying $\mathbf{V}^{(i)}$ to $\mathbf{Q}^{(i+1)}$ factors.   */

11 **for** $i = L - 1 : -1 : 1$ **do**

12   **for** $j = 1 : 2^{L-i}$ **do**

13          $\mathbf{Q}^{(i)}_j \leftarrow \texttt{hh\_mult}\left(\mathbf{V}^{(i)}_j, \begin{bmatrix} \tilde{\mathbf{Q}}^{(i+1)}_{\alpha(j),\phi(j)} \\ \mathbf{0} \end{bmatrix} \right)$

14 $\mathbf{Q} \leftarrow []$;   // Construct the final Q factor.

15 **for** $j = 1 : 2^L$ **do**

16      $\mathbf{Q} \leftarrow \begin{bmatrix} \mathbf{Q} \\ \texttt{hh\_mult}\left(\mathbf{V}^{(0)}_j, \begin{bmatrix} \tilde{\mathbf{Q}}^{(1)}_{\alpha(j),\phi(j)} \\ \mathbf{0} \end{bmatrix} \right) \end{bmatrix}$

17 **return** $\mathbf{Q}, \mathbf{R}$

3.3.2. Single-level Example. In the single-level version of this algorithm, we first bisect $\mathbf{A}$ into $\mathbf{A}^{(0)}_1$ and $\mathbf{A}^{(0)}_2$ 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:

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

18

567 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,
568 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 $\tilde{\mathbf{Q}}_{1,2}^{(1)}$,
569 allows us to write and compute the product more compactly,

$$570 \qquad \mathbf{Q} := \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \mathbf{Q}_1^{(1)} = \begin{bmatrix} \mathbf{Q}_1^{(0)} & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_2^{(0)} \end{bmatrix} \begin{bmatrix} \tilde{\mathbf{Q}}_{1,1}^{(1)} \\ \tilde{\mathbf{Q}}_{1,2}^{(1)} \end{bmatrix} = \begin{bmatrix} \mathbf{Q}_1^{(0)} \tilde{\mathbf{Q}}_{1,1}^{(1)} \\ \mathbf{Q}_2^{(0)} \tilde{\mathbf{Q}}_{1,2}^{(1)} \end{bmatrix}.$$

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

578 **3.3.3. TSQR: Rounding Error Analysis.** The TSQR algorithm presented in alg. 6 is a
579 divide-and-conquer strategy for the QR factorization that uses the HQR within the subproblems.
580 Divide-and-conquer methods can naturally be implemented in parallel and accumulate less rounding
581 errors. For example, the single-level TSQR decomposition of a tall-and-skinny matrix, $\mathbf{A}$ requires
582 3 total HQRs of matrices of sizes $\lfloor \log_2(\frac{m}{n}) \rfloor$-by-$n$, $\lceil \log_2(\frac{m}{n}) \rceil$-by-$n$, and $2n$-by-n. The single-level
583 TSQR strictly uses more FLOPs, but the dot product subroutines may accumulate smaller rounding
584 errors (and certainly have smaller upper bounds) since they are performed on shorter vectors, and
585 lead to a more accurate solution overall. These concepts are elucidated in [18] and we summarize
586 the main results in Theorem 3.7.

587 THEOREM 3.7. *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*
588 *the thin QR factors of* $\mathbf{A}$ *obtained via* alg. 6 *with* L *levels. Let us further assume that* m *is divisible*
589 *by* 2^L *and* $n\tilde{\gamma}_{m2^{-L}}, n\tilde{\gamma}_{2n} \ll 1$. *Then, normwise error bounds for the* j^{th} *column* ($j = 1 : n$) *are*

590 (3.26) $$\|\hat{\mathbf{R}}_{TSQR}[:,j] - \mathbf{R}[:,j]\|_2 \leq n(\tilde{\gamma}_{m2^{-L}} + L\tilde{\gamma}_{2n})\|\mathbf{A}[:,j]\|_2,$$

591 (3.27) $$\|\hat{\mathbf{Q}}_{TSQR}[:,j] - \mathbf{Q}[:,]\|_2 \leq n(\tilde{\gamma}_{m2^{-L}} + L\tilde{\gamma}_{2n}).$$
592

593 Note that the $n\tilde{\gamma}_{m2^{-L}}$ and $n\tilde{\gamma}_{2n}$ terms correspond to errors from applying HQR to the blocks
594 in the initial partition and to the blocks in levels 1 through L respectively. We can easily replace
595 these with analogous mixed precision terms and keep the analysis accurate. Both level-2 and level-3
596 BLAS implementations will be considered in section 4.

597 **4. Mixed precision error analysis.** Let us first consider rounding errors incurred from
598 carrying out HQR in high precision, then cast down at the very end. This could be useful in
599 applications that require economical storage but have enough memory to carry out HQR in higher
600 precision, or in block algorithms as will be shown in subsections 4.1 and 4.2. Consider two floating
601 point types $\mathbb{F}_l$ and $\mathbb{F}_h$ where $\mathbb{F}_l \subseteq \mathbb{F}_h$, and for all $x, y \in \mathbb{F}_l$, the exact product xy can be represented
602 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
603 that the matrix to be factorized is stored with low precision numbers, $\mathbf{A} \in \mathbb{F}_l^{m \times n}$. Casting up
604 adds no rounding errors, so we can directly apply the analysis that culminated in Theorem 3.4,
605 and we only consider the columnwise forward error in the $\mathbf{Q}$ factor. Then, the jth column of
606 $\hat{\mathbf{Q}}_{HQR} = \mathbf{Q} + \Delta\mathbf{Q}_{HQR}$ is bounded normwise via $\|\Delta\mathbf{Q}_{HQR}[:,j]\|_2 \leq n\tilde{\gamma}_m^h$, and incurs an extra
607 rounding error when $\mathbf{Q} \in \mathbb{F}_h^{m \times n}$ is cast down to $F_l^{m \times n}$.

19

First, consider casting down a higher precision number $x \in \mathbb{F}_h$ to $\mathbb{F}_l$ without overflow. We result in

$$\texttt{castdown}(x) = x(1 + \delta^{(l)}), \;\; |\delta^{(l)}| < u^{(l)},$$

and accrues a single rounding error in the lower precision. Extending this result, we represent the backward error of a casting down a vector in $\mathbb{F}_h^{(m)}$ with a linear transformation, $\mathbf{I}^{(l)} \in \mathbb{R}^{m \times m}$. This transformation is a diagonal perturbation of the identity, $\mathbf{I}_m$. For some vector $\mathbf{x} \in \mathbb{F}_h$, the cast down operation yields

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

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 (3.12) to form a backward matrix norm bound,

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

Using this in Lemma 3.2 to analyze the forward norm error for the jth column of the $\mathbf{Q}$ factor computed with alg. 3 yields

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

Similarly, we can apply the operator $\mathbf{I}^{(l)}$ to cast down any quantity stored in the higher precision. If BQR and TSQR were computed entirely in the higher precision then cast down at the end, then the corresponding forward matrix norm errors on the $\mathbf{Q}$ factor are

$$\|\hat{\mathbf{Q}}_{BQR}\|_F \leq u^{(l)} + n\tilde{\gamma}_m^{(h)} + u^{(l)}n\tilde{\gamma}_m^{(h)},$$
$$\|\hat{\mathbf{Q}}_{TSQR}\|_F \leq u^{(l)} + n(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2^{-L}}^{(h)}) + u^{(l)}n(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2^{-L}}^{(h)}).$$

We will modify BQR and TSQR so that matrix-matrix multiply and accumulate operations can be performed on TensorCore block FMAs which work on 4-by-4 matrices, $\mathbf{A}, \mathbf{B}, \mathbf{C},$, and $\mathbf{D}$ that compute

$$\mathbf{D} = \text{fl}(\mathbf{C} + \mathbf{AB}),$$

where $\mathbf{A}, \mathbf{B} \in \mathbb{F}_{\text{fp16}}^{4 \times 4}$ and $\mathbf{C}, \mathbf{D} \in \mathbb{F}_{\text{fp16}}^{4 \times 4}$ or $\mathbf{C}, \mathbf{D} \in \mathbb{F}_{\text{fp32}}^{4 \times 4}$. The inner product step in forming $\mathbf{AB}$ is similar to Assumption 2.3 in that full precision (exact) products are accumulated in the higher precision, fp32. One difference is that the cast down operation at the end of the inner product is optional. Matrices larger than 4-by-4's can be multiplied and added using this optional cast down feature and by using block matrix multiplication with 4-by-4 blocks. In subsection 4.1, we consider performing BQR and TSQR with high precision FLOPs within a block/level, but cast down to low precision in between blocks and at the very end. Finally, in subsection 4.2, we consider all 3 algorithms with the ad hoc mixed precision setting described in Assumption 2.3 where inner products are performed in high precision before being cast down, and all other operations are computed in low precision.

4.1. Round down at block-level (BLAS-3). We directly apply (4.3) to all instances of HQR to the error analyses for BQR and TSQR in section 3. Therefore, a cast down operation should occur at every block/level and the insertion of low precision errors $u^{(l)}$ should be somewhat correlated to the number of blocks and levels.

20

646 **4.1.1. Round down at block level: BQR.** Consider the input matrix, $\mathbf{A} \in \mathbb{F}_l^{m \times n}$, parti-
647 tioned into N blocks of r columns, $\mathbf{A} = [\mathbf{C}_1 \cdots \mathbf{C}_N]$ as was in the analysis in subsection 3.2. We
648 assume that the returned factors should also be represented in the lower precision, $\mathbb{F}_l$, and modify
649 alg. 5 so that matrix-matrix multiply and accumulate operations are performed with TensorCore
650 block FMAs. Since approximately $\mathcal{O}(1/N)$ (small) fraction of FLOPs are performed in level-1 and
651 level-2 BLAS operations, we assume that we can afford to compute these in high precision. Let us
652 store the $\mathbf{R}$ factor from each call to HQR in low precision, and keep the Householder constants and
653 vectors $(\boldsymbol{\beta}_k^{(j)}, \mathbf{v}_k^{(j)})$in high precision to build the WY representation. Since the WY representations
654 $(\mathbf{W}_k, \mathbf{V}_k)$ should be stored in low precision, we enforce a cast down at the end of alg. 4. Finally, all
655 but the last WY update for each block are stored in the higher precision, and the last WY update
656 returned in low precision. This mixed precision BQR variant is rich in level-3 BLAS operations can
be implemented with TensorCore block FMAs easily, and is formally introduced in alg. 7.

Algorithm 7: $\hat{\mathbf{Q}}_{mpBQR}, \hat{\mathbf{R}}_{mpBQR} \leftarrow \texttt{mpBQR}(\mathbf{A}, r)$: Perform Householder QR factoriza-
tion of matrix $\mathbf{A}$ with column partitions of size r. All inputs and outputs are stored in
low precision. Matrix-matrix multiplication and accumulate operations in lines 10, 13,
and 14 require low precision inputs but can return in either of the two precisions.

Input: $\mathbf{A} \in \mathbb{F}_l^{m \times n}$, $r \in \mathbb{R}$ where $n = Nr$.
Output: $\mathbf{Q} \in \mathbb{F}_l^{m \times n}, \mathbf{R} \in \mathbb{F}_l^{n \times n}$
1 $N = \frac{n}{r}$
   // Let $\mathbf{A} = [\mathbf{C}_1 \cdots \mathbf{C}_N]$ where all blocks except $\mathbf{C}_N$ are m-by-r sized.
2 **for** $k = 1 : N - 1$ **do**
3   **if** $k == 1$ **then**
4        $\mathbf{V}_1, \boldsymbol{\beta}_1, \mathbf{C}_1 \leftarrow \texttt{hhQR}(\texttt{castup}(\mathbf{C}_k))$ /* Algorithm 3 in high precision. */
5   **else**
6        $\mathbf{V}_k, \boldsymbol{\beta}_k, \mathbf{C}_k \leftarrow \texttt{hhQR}(\mathbf{C}_k)$ /* Algorithm 3 in high precision. */
7     $\mathbf{C}_k \leftarrow \texttt{castdown}\ (\mathbf{C}_k)$ /* Builds $\mathbf{R}$ factor in low precision. */
8     $\mathbf{W}_k \leftarrow \texttt{buildWY}(\mathbf{V}_k, \boldsymbol{\beta}_k)$ /* Algorithm 4 in high precision */
9     $[\mathbf{V}_k, \mathbf{W}_k] \leftarrow \texttt{castdown}([\mathbf{V}_k, \mathbf{W}_k])$
10    $[\mathbf{C}_{k+1} \cdots \mathbf{C}_N] \mathrel{-}= \mathbf{V}_k \left(\mathbf{W}_k^\top [\mathbf{C}_{k+1} \cdots \mathbf{C}_N]\right)$ /* returned in low precision */
   // Now build $\mathbf{Q}$ using level-3 BLAS operations.
11 $\mathbf{Q} \leftarrow \mathbf{I}$ /* $\mathbf{I}_m$ if full QR, and $\mathbf{I}_{m \times n}$ if thin QR. */
12 **for** $k = N : -1 : 1$ **do**
   // All updates are returned in low precision.
13     $\mathbf{Q}[(k-1)r + 1 : m, (k-1)r + 1 : n] \mathrel{-}= \mathbf{W}_k \left(\mathbf{V}_k^\top \mathbf{Q}[(k-1)r + 1 : m, (k-1)r + 1 : n]\right)$
14 **return** $\mathbf{Q}, \mathbf{A}$

657
658   Since $\hat{\mathbf{W}}_k, \hat{\mathbf{Y}}_k$'s are computed with alg. 4 then cast down, the low precision WY update is
659 $\hat{\mathbf{X}}_k^{(l)} = \mathbf{I} - \mathbf{I}^{(l)} \hat{\mathbf{W}}_k \mathbf{I}^{(l)} \hat{\mathbf{V}}_k^{(\top)}$. Consider applying $\hat{\mathbf{X}}_k^{(l)}$ to some matrix stored in low precision, $\mathbf{B}$ using
660 the TensorCore block FMAs. We analyze a single column $\mathbf{b}_j := \mathbf{B}[:, j] \in \mathbb{F}_l^{m-(k-1)r}$ even though
661 this operation is done on $\mathbf{B}$ as a whole. Let $\mathbf{I}^{(l)} \hat{\mathbf{W}}_k = \hat{\mathbf{W}}_k + \mathbf{E}_W \hat{\mathbf{W}}_k$ and $\mathbf{I}^{(l)} \hat{\mathbf{W}}_k = \hat{\mathbf{Y}}_k + \mathbf{E}_Y \hat{\mathbf{Y}}_k$,

21

where $|\mathbf{E}_W|, |\mathbf{E}_Y| \leq u^{(l)}$ componentwise. Since

$$\hat{\mathbf{X}}_k^{(l)} - \mathbf{X}_k = \hat{\mathbf{X}}_k^{(l)} - \hat{\mathbf{X}}_k + \hat{\mathbf{X}}_k - \mathbf{X}_k = \hat{\mathbf{X}}_k^{(l)} - \hat{\mathbf{X}}_k + \Delta\mathbf{X}_k,$$

we only need to add the errors introduced from casting down to the errors derived in (3.17),

$$\|(\hat{\mathbf{X}}_k^{(l)} - \hat{\mathbf{X}}_k + \Delta\mathbf{X}_k)\mathbf{b}_j\|_2 = \|\left(-\left(\mathbf{E}_W + \mathbf{E}_Y + \mathbf{E}_W\mathbf{E}_Y\right)\hat{\mathbf{W}}_k\hat{\mathbf{Y}}_k^\top + \Delta\mathbf{X}_k\right)\mathbf{b}_j\|_2,$$

$$= (\gamma_2^{(l)}(1 + r\tilde{\gamma}_{m-(k-1)r}^{(h)}) + r\tilde{\gamma}_{m-(k-1)r}^{(h)})\|\mathbf{b}_j\|_2.$$

Therefore, we have $\|(\hat{\mathbf{X}}_k^{(l)} - \mathbf{X}_k)\mathbf{b}_j\|_2 \leq (\gamma_2^{(l)} + r\tilde{\gamma}_{m-(k-1)r}^{(h)} + r\gamma_2^{(l)}\tilde{\gamma}_{m-(k-1)r}^{(h)})\|\mathbf{b}_j\|_2$ and the error bound on the corresponding backward matrix norm is

$$(4.4) \qquad \|\Delta^{(l)}\mathbf{X}_k\|_F \leq \gamma_2^{(l)} + r\tilde{\gamma}_{m-(k-1)r}^{(h)} + r\gamma_2^{(l)}\tilde{\gamma}_{m-(k-1)r}^{(h)},$$

where $\Delta^{(l)}\mathbf{X}_k = \hat{\mathbf{X}}_k^{(l)} - \mathbf{X}_k$.

We can finally compute the forward errors on the QR factorization computed via alg. 7. Consider the jth column of the $\mathbf{Q}$ factor, which we denote with $\mathbf{q}_j := \hat{\mathbf{Q}}_{mpBQR}[:,j]$, and let $k = \lfloor j/r \rfloor$. for $k' = 1 : N$, and (4.4) was used to invoke Lemma 3.2. Then the columnwise error is

$$(4.5) \qquad \|\Delta\mathbf{q}_j\|_2 \leq -1 + \prod_{k'=1}^k (1 + \gamma_2^{(l)})(1 + r\tilde{\gamma}_{m-(k'-1)r}^{(h)})$$

$$(4.6) \qquad \leq k\gamma_2^{(l)} + kr\tilde{\gamma}_m^{(h)} + k^2 r\gamma_2^{(l)}\tilde{\gamma}_m^{(h)},$$

where $\Delta\mathbf{q}_j = (\hat{\mathbf{X}}_1^{(l)} \cdots \hat{\mathbf{X}}_k^{(l)} - \mathbf{X}_1 \cdots \mathbf{X}_k)\hat{e}_j$. Summing over the columns to find a matrix norm error bound yields

$$(4.7) \qquad \|\hat{\mathbf{Q}}_{mpBQR} - \mathbf{Q}\|_F \leq n^{1/2}\tilde{\gamma}_N^{(l)} + n^{(3/2)}\tilde{\gamma}_m^{(h)},$$

where the summation of the third term in (4.6) is swept under the tilde notation in $n^{1/2}\tilde{\gamma}_N^{(l)}$. This bound shows that alg. 7 only adds $n^{1/2}\tilde{\gamma}_N^{(l)}$ order errors to the bounds in (3.25). Using that $u^{(l)} = M_{l,h}u^{(h)}$, this increase corresponds to a multiplicative factor shown below,

$$(4.8) \qquad n^{1/2}\tilde{\gamma}_N^{(l)} + n^{(3/2)}\tilde{\gamma}_m^{(h)} \approx \left(1 + \frac{M_{l,h}}{rm}\right)n^{(3/2)}\tilde{\gamma}_m^{(h)}.$$

Therefore, the loss in accuracy due to mixed precision computing is relatively small when the disparity in precision ($M_{l,h}$) is small in comparison to the block size, mr. Whether this loss in accuracy in the worst-case scenario is worth the speed-ups from using mixed precision hardware is an open question that can be tackled in future research. We expect that the block size r, the dimension of the input matrix m, n, and hardware specificities will be contributing factors.

4.1.2. Round down at block level: TSQR. Let us now consider a variant of TSQR, where all instances of `hh_mult` are replaced by some level-3 BLAS operations. Note that for all blocks in all levels, exactly n Householder transformations of lengths either $m2^{-L}$ or $2n$ are applied via `hh_mult`. Let $\tilde{m} := \max\{m2^{-L}, 2n\}$ be the larger of the two. We consider two ways of applying n Householder transformations with level-3 BLAS operations.

22

1. Consider building the WY representation using high precision arithmetic, casting them down and then applying the update with TensorCore block FMAs. The multiplication by the $\mathbf{Y}$ factor requires at most $\tilde{m}$-length inner products and a cast down operation and the multiplication by the $\mathbf{W}$ factor requires n-length inner products and another cast down operation. The errors accumulated from these actions are bounded by $\mathcal{O}(3u^{(l)} + \tilde{\gamma}_{\tilde{m}n}^{(h)})$ componentwise.

2. Now, consider applying the n Householder transformations by forming the operator explicitly then computing a single matrix-matrix product. We form the operator using the same steps as forming the $\mathbf{Q}$ factor in HQR in high precision arithmetic, then cast the result down. The construction of the operator and the cast down result in error bounded by $\mathcal{O}(u^{(l)} + \tilde{\gamma}_{\tilde{m}n}^{(h)})$, and the matrix-matrix product requires $\tilde{m}$-length inner products and another cast down operation. This option also accrues error bounded by $\mathcal{O}(2u^{(l)} + \tilde{\gamma}_{\tilde{m}n}^{(h)})$.

Both of these options require more FLOPs than in the standard algorithm implemented with level-2 BLAS operations, since the same number of level-2 BLAS operations are required to form the matrices required for the level-3 variants. The level-3 variants are built during the formation of the $\mathbf{R}$ factor and can be reused when forming the $\mathbf{Q}$ factor. Notice that unlike BQR which is rich in level-3 BLAS operations by design, it is not clear whether implementing TSQR with level-3 BLAS operations has obvious benefits. Regardless, we still perform a rounding error analysis of TSQR performed with mixed precision level-3 BLAS operations, i.e. TensorCore block FMAs.

The analysis in [18] shows that each column of $\mathbf{Q}$ is transformed by n Householder transformations of length $2n$ from levels $L : -1 : 1$, and another set of n Householder transformations of length $m2^{-L}$ at level 0. We can easily modify the analysis in [18] and applying Lemma 3.2 by adding $(1 + 2u^{(l)})$ to every set of n Householder transformations in each level. There are two low precision rounding errors in each block per level since casting down the matrix operator formed with high precision is cast down to the low precision, and the matrix-matrix product used in applying this operator with TensorCore block FMAs incurs another low precision rounding error. Therefore, all instances of $n\tilde{\gamma}_{m2^{-L}}, n\tilde{\gamma}_{2n}$ are replaced with

$$(1 + 2u^{(l)})(1 + n\tilde{\gamma}_{m2^{-L}}^{(h)}) - 1, \quad \text{and} \quad (1 + 2u^{(l)})(1 + n\tilde{\gamma}_{2n}^{(h)}) - 1.$$

Then, the $\mathbf{Q}$ factor formed with this mixed precision variant of TSQR is denoted with $\hat{\mathbf{Q}}_{mpTSQR}$ and its jth column has rounding errors bounded by,

$$(4.9) \qquad \|\hat{\mathbf{Q}}_{mpTSQR}[:, j] - \mathbf{Q}[:, j]\|_2 \le \tilde{\gamma}_{L+1}^{(l)} + n\left(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2^{-L}}^{(h)}\right).$$

Summing up the columns for a matrix norm error bound, we result in

$$(4.10) \qquad \|\hat{\mathbf{Q}}_{mpTSQR} - \mathbf{Q}\|_F \le n^{1/2}\tilde{\gamma}_{L+1}^{(l)} + n^{3/2}\left(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2^{-L}}^{(h)}\right).$$

Therefore, we can convert the additional low precision rounding errors into a multiplicative factor of the original bound in (3.27),

$$(4.11) \qquad n^{1/2}\tilde{\gamma}_{L+1}^{(l)} + n^{3/2}\left(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2^{-L}}^{(h)}\right) = (1 + \frac{M_{l,h}L}{n(2nL + m2^{-L})})n^{3/2}\left(L\tilde{\gamma}_{2n}^{(h)} + \tilde{\gamma}_{m2^{-L}}^{(h)}\right).$$

Once again, the constant that represents the disparity in the two precisions, $M_{l,h}$ is compared against the original matrix size m, n and the block size specifications defined by 2^L and the number of levels, L.

23

4.2. Round down at inner-product. While the previous section discussed blocked variants of HQR that can be easily adapted for the mixed precision setting specific to TensorCore's level-3 BLAS operations, we want to provide a more general mixed precision environment in this section. Recall that HQR, BQR, and TSQR all rely on Householder transformations in one way or another, and Householder transformations are essentially performed via (3.9). This implementation capitalizes on the rank-1 update structure of Householder transformations where the predominant share of FLOPs is spent on an inner product, and computing the Householder vector and constant also rely heavily on inner products. Therefore, we can attribute nearly all of the computational tasks for algs. 3, 5 and 6 to the inner product. In addition, the inner product is just as important in non-HQR linear algebra tools, where some examples include projections and matrix-vector, matrix-matrix multiply. Consequently, we return to the mixed precision setting described in section 2, where every inner product is cast down to the lower precision as shown in (2.11).

4.2.1. Round down at inner product: HQR. Consider forming a Householder transformation that zeros out $\mathbf{x} \in \mathbb{R}^m$ below the the ith element. We need to compute σ, β, $\tilde{\mathbf{v}}_1$, and $\mathbf{v}$ as defined in subsection 3.1:

$$(4.12) \qquad \mathrm{fl}(\sigma) = \mathrm{fl}(-\mathrm{sign}(\mathbf{x}[1])\|\mathbf{x}\|_2) = \sigma + \Delta\sigma, \;\; |\Delta\sigma| \leq (\gamma_2^{(\mathrm{l})} + \gamma_{\mathrm{m}}^{(\mathrm{h})} + \gamma_2^{(\mathrm{l})}\gamma_{\mathrm{m}}^{(\mathrm{h})})|\sigma|,$$

$$(4.13) \qquad \mathrm{fl}(\tilde{\mathbf{v}}[1]) = \tilde{\mathbf{v}}[1] + \Delta\tilde{\mathbf{v}}[1] = (1 + \delta^{(l)})(\mathbf{x}[1] - \sigma - \Delta\sigma), \;\; |\Delta\tilde{\mathbf{v}}[1]| \leq (\gamma_3^{(l)} + \tilde{\gamma}_m^{(h)})|\tilde{\mathbf{v}}[1]|$$

$$(4.14) \qquad \mathrm{fl}(\beta) = \beta + \Delta\beta = (1 + \delta^{(l)})(-\tilde{\mathbf{v}}[1]/\hat{\sigma}), \;\; |\Delta\beta| \leq (\gamma_8^{(l)} + \tilde{\gamma}_m^{(h)})|\beta|,$$

$$(4.15) \qquad \mathrm{fl}(\mathbf{v}[j]) = \mathbf{v}[j] + \Delta\mathbf{v}[j] \text{ where } |\Delta\mathbf{v}_j| \leq \begin{cases} 0, & j = 1 \\ (\gamma_7^{(l)} + \tilde{\gamma}_m^{(h)})|\mathbf{v}_j|, & j = 2 : m - i + 1. \end{cases}$$

These bounds on $\Delta\sigma$, $\Delta\tilde{\mathbf{v}}[1]$, $\Delta\beta$, and $\Delta\mathbf{v}[j]$ are computed by using the rules from Lemma 2.4 on the analysis shown in subsection 3.1. Using these, we can formulate the mixed precision version of (3.10) where $\hat{\mathbf{y}} = \mathrm{fl}(\mathbf{P_v}\mathbf{x}) \in \mathbb{R}^m$ is implemented via (3.9). Note that the inner product $\hat{\mathbf{v}}^\top\mathbf{x}$ is computed with the mixed precision inner product scheme outlined in Assumption 2.3, and all other operations are done in the lower precision. Then, the transformed vector is bounded by

$$(4.16) \qquad \hat{\mathbf{y}} = \mathbf{y} + \Delta\mathbf{y}, \;\; \|\Delta\mathbf{y}\|_2 \leq (\gamma_{25}^{(l)} + \tilde{\gamma}_m^{(h)})\|\mathbf{y}\|_2.$$

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

$$(4.17) \qquad \hat{\mathbf{y}} = (\mathbf{P_v} + \Delta\mathbf{P_v})\mathbf{x}, \;\; \|\Delta\mathbf{P_v}\|_F \leq (\gamma_{25}^{(l)} + \tilde{\gamma}_m^{(h)}).$$

Now, we form the error bounds for applying n Householder transformations to $\mathbf{x}$ using Lemma 3.2,

$$(4.18) \qquad \hat{\mathbf{y}} = \mathbf{Q}(\mathbf{x} + \Delta\mathbf{x}) = (\mathbf{Q} + \Delta\mathbf{Q})\mathbf{x},$$

$$(4.19) \qquad \|\Delta\mathbf{y}\|_2 \leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)})\|\mathbf{x}\|_2, \;\; \|\Delta\mathbf{Q}\|_F \leq (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}).$$

Note that we have additionally assumed that $25 \ll n$ and used the $\tilde{\gamma}^{(l)}$ notation. The analogous mixed precision QR factorization error bounds are shown in Theorem 4.1.

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* $\hat{\mathbf{R}} \in \mathbb{R}^{n \times n}_{mpHQR}$ *be the thin QR factors of* $\mathbf{A}$ *obtained via* alg. 3 *with mixed precision FLOPs where*

24

inner products are computed in precision h then cast down. All other operations are carried out in precision l. Then,

$$\|\Delta \mathbf{R}_{mpHQR}[:,j]\|_2 \le (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)})\|\mathbf{A}[:,j]\|_2, \quad \|\Delta \mathbf{R}_{mpHQR}\|_F \le (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)})\|\mathbf{A}\|_F$$

$$\|\Delta \mathbf{Q}[:,j]_{mpHQR}\|_2 \le (\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}), \quad \|\Delta \mathbf{Q}_{mpHQR}\|_F \le n^{1/2}(\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_m^{(h)}).$$

4.2.2. Round down at inner product: BQR. Now, we analyze alg. 5 with the mixed precision inner product scheme of Assumption 2.3. At the kth block, we first apply the mixed precision HQR summarized in Theorem 4.1. Next, we construct the WY representation, where we can now use (4.16) and (4.17) and Lemma 3.2 to form

(4.20) $$\|\hat{\mathbf{X}}_k^{(l)} - \mathbf{X}_k\|_F = \|(\hat{\mathbf{P}}_k^{(1)} \cdots \hat{\mathbf{P}}_k^{(r)}) - (\mathbf{P}_k^{(1)} \cdots \mathbf{P}_k^{(r)})\|_F \le \tilde{\gamma}_r^{(l)} + r\tilde{\gamma}_m^{(h)}.$$

Then, the jth column of the $\mathbf{Q}$ factor resulting from this mixed precision variant of BQR incurs rounding errors bounded by

(4.21) $$\|\hat{\mathbf{Q}}_{mpBQR2}[:,j]\|_F = \|\hat{\mathbf{X}}_1 \cdots \hat{\mathbf{X}}_N \hat{e}_j\|_2 \le N\tilde{\gamma}_r^{(l)} + n\tilde{\gamma}_m^{(h)},$$

and the matrix norm error bound is,

(4.22) $$\|\hat{\mathbf{Q}}_{mpBQR2}\|_F \le n^{1/2}N\tilde{\gamma}_r^{(l)} + n^{3/2}\tilde{\gamma}_m^{(h)} \approx (1 + \frac{M_{l,h}}{m})n^{3/2}\tilde{\gamma}_m^{(h)}.$$

Recall that the block mixed precision variant of section 4.1.1 yielded a multiplicative factor of $(1 + \frac{M_{l,h}}{rm})$ (see (4.8)). This implies that the mixed precision inner product introduces low precision error $r\times$ larger than the low precision errors incurred from casting down at the block level. However, if m is sufficiently larger than $M_{l,h}$, the mixed precision inner product can still had non-leading order error terms to the worst-case scenario.

4.2.3. Round down at inner product: TSQR. Finally, we consider using the mixed precision inner product of Assumption 2.3 in alg. 6. This corresponds to replacing every instance of $n\tilde{\gamma}_{m'}$ for $m' \in \{2n, m2^{-L}\}$ in Theorem 3.7 with $\tilde{\gamma}_n^{(l)} + n\tilde{\gamma}_{m'}^{(h)}$. We first consider the norm errors for the jth column of the $\mathbf{Q}$ factor computed by this mixed precision variant of alg. 6,

(4.23) $$\|\hat{\mathbf{Q}}_{mpTSQR2}[:,j] - \mathbf{Q}[:,j]\|_2 \le (L+1)\tilde{\gamma}_n^{(l)} + n(\tilde{\gamma}_{m2^{-L}}^{(h)} + L\tilde{\gamma}_{2n}^{(h)}).$$

Then, the matrix norm error bound is

(4.24) $$\|\hat{\mathbf{Q}}_{mpTSQR2} - \mathbf{Q}\|_F \le n^{1/2}(L+1)\tilde{\gamma}_n^{(l)} + n^{3/2}(\tilde{\gamma}_{m2^{-L}}^{(h)} + L\tilde{\gamma}_{2n}^{(h)})$$

(4.25) $$\approx \left(1 + \frac{M_{l,h}L}{m2^{-L} + 2Ln}\right)n^{3/2}(\tilde{\gamma}_{m2^{-L}}^{(h)} + L\tilde{\gamma}_{2n}^{(h)}).$$

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.

25

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.

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.

REFERENCES

[1] A. ABDELFATTAH, S. TOMOV, AND J. DONGARRA, *Fast batched matrix multiplication for small sizes using half-precision arithmetic on GPUs*, in 2019 IEEE International Parallel and Distributed Processing Symposium (IPDPS), May 2019, pp. 111–122, https://doi.org/10.1109/IPDPS.2019.00022.

[2] J. APPLEYARD AND S. YOKIM, *Programming Tensor Cores in CUDA 9*, 2017, https://devblogs.nvidia.com/programming-tensor-cores-cuda-9/ (accessed 2018-07-30).

[3] G. BALLARD, J. W. DEMMEL, L. GRIGORI, M. JACQUELIN, H. DIEP NGUYEN, AND E. SOLOMONIK, *Reconstructing Householder vectors from tall-skinny QR*, vol. 85, 05 2014, pp. 1159–1170, https://doi.org/10.1109/IPDPS.2014.120.

[4] C. BISCHOF AND C. VAN LOAN, *The WY Representation for Products of Householder Matrices*, SIAM Journal on Scientific and Statistical Computing, 8 (1987), pp. s2–s13, https://doi.org/10.1137/0908009.

[5] M. COURBARIAUX, Y. BENGIO, AND J.-P. DAVID, *Training deep neural networks with low precision multiplications*, arXiv preprint, arXiv:1412.7024, (2014).

[6] M. COURBARIAUX, J.-P. DAVID, AND Y. BENGIO, *Low precision storage for deep learning*, arXiv preprint arXiv:1412.7024, (2014).

[7] J. DEMMEL, I. DUMITRIU, AND O. HOLTZ, *Fast linear algebra is stable*, Numerische Mathematik, 108 (2007), pp. 59–91, https://doi.org/10.1007/s00211-007-0114-x, https://arxiv.org/abs/0612264.

[8] J. DEMMEL, L. GRIGORI, M. HOEMMEN, AND J. LANGOU, *Communication-optimal parallel and sequential QR and LU factorizations*, SIAM Journal on Scientific Computing, 34 (2012), https://doi.org/10.1137/080731992, https://arxiv.org/abs/0808.2664.

[9] G. H. GOLUB AND C. F. VAN LOAN, *Matrix computations*, JHU press, 4 ed., 2013.

[10] A. HAIDAR, A. ABDELFATTAH, M. ZOUNON, P. WU, S. PRANESH, S. TOMOV, AND J. DONGARRA, *The Design of Fast and Energy-Efficient Linear Solvers: On the Potential of Half-Precision Arithmetic and Iterative Refinement Techniques*, June 2018, pp. 586–600, https://doi.org/10.1007/978-3-319-93698-7_45.

[11] A. HAIDAR, S. TOMOV, J. DONGARRA, AND N. J. HIGHAM, *Harnessing GPU tensor cores for fast fp16 arithmetic to speed up mixed-precision iterative refinement solvers*, in Proceedings of the International Conference for High Performance Computing, Networking, Storage, and Analysis, SC '18, Piscataway, NJ, USA, 2018, IEEE Press, pp. 47:1–47:11, https://doi.org/10.1109/SC.2018.00050, https://doi.org/10.1109/SC.2018.00050.

[12] N. J. HIGHAM, *Accuracy and Stability of Numerical Methods*, 2002, https://doi.org/10.2307/2669725.

[13] N. J. HIGHAM AND T. MARY, *A New Approach to Probabilistic Rounding Error Analysis*, SIAM Journal on Scientific Computing, 41 (2019), pp. A2815–A2835, https://doi.org/10.1137/18M1226312, https://epubs.siam.org/doi/10.1137/18M1226312.

26

[14] N. J. HIGHAM AND S. PRANESH, *Simulating Low Precision Floating-Point Arithmetic*, SIAM Journal on Scientific Computing, 41 (2019), pp. C585–C602, https://doi.org/10.1137/19M1251308, https://epubs.siam.org/doi/10.1137/19M1251308.

[15] A. S. HOUSEHOLDER, *Unitary triangularization of a nonsymmetric matrix*, Journal of the ACM (JACM), 5 (1958), pp. 339–342.

[16] I. C. F. IPSEN AND H. ZHOU, *Probabilistic Error Analysis for Inner Products*, (2019), http://arxiv.org/abs/1906.10465, https://arxiv.org/abs/1906.10465.

[17] P. MICIKEVICIUS, S. NARANG, J. ALBEN, G. DIAMOS, E. ELSEN, D. GARCIA, B. GINSBURG, M. HOUSTON, O. KUCHAIEV, G. VENKATESH, AND H. WU, *Mixed precision training*, in International Conference on Learning Representations, 2018, https://openreview.net/forum?id=r1gs9JgRZ.

[18] D. MORI, Y. YAMAMOTO, AND S. L. ZHANG, *Backward error analysis of the AllReduce algorithm for householder QR decomposition*, Japan Journal of Industrial and Applied Mathematics, 29 (2012), pp. 111–130, https://doi.org/10.1007/s13160-011-0053-x.

[19] R. SCHREIBER AND C. VAN LOAN, *A Storage-Efficient WY Representation for Products of Householder Transformations*, SIAM Journal on Scientific and Statistical Computing, 10 (1989), pp. 53–57, https://doi.org/10.1137/0910005.

[20] G. TAGLIAVINI, S. MACH, D. ROSSI, A. MARONGIU, AND L. BENIN, *A transprecision floating-point platform for ultra-low power computing*, in 2018 Design, Automation Test in Europe Conference Exhibition (DATE), March 2018, pp. 1051–1056, https://doi.org/10.23919/DATE.2018.8342167.

27