Householder orthogonalization with a non-standard inner product

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Abstract

Householder orthogonalization plays an important role in numerical linear algebra. It attains perfect orthogonality regardless of the conditioning of the input. However, in the context of a non-standard inner product, it becomes difficult to apply Householder orthogonalization due to the lack of an initial orthonormal basis. We propose strategies to overcome this obstacle and discuss algorithms and variants of Householder orthogonalization with a non-standard inner product. Theoretical analysis and numerical experiments demonstrate that our approach is numerically stable under mild assumptions.

Keywords: Householder reflection, orthonormal basis, QR factorization, Gram–Schmidt process, non-standard inner product

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1 Introduction

Let $B \in \mathbb{C}^{n \times n}$ be Hermitian and positive definite, and $X \in \mathbb{C}^{n \times k}$ with $n \geq k$. There exist $Q \in \mathbb{C}^{n \times k}$ and an upper triangular matrix $R \in \mathbb{C}^{k \times k}$ such that

$$X = QR, \quad (1)$$
$$Q^H B Q = I_k. \quad (2)$$

The factorization (1) is known as a thin QR factorization [7] or a reduced QR factorization [22] of the matrix $X$. Condition (2) means that the columns of $Q$ form an orthonormal basis of span$(Q)$ in the non-standard inner product $\langle u, v \rangle_B = v^H B u$ induced by $B$, where the superscript $^H$ stands for the conjugate transpose of a matrix. Throughout this paper we call $\langle \cdot, \cdot \rangle_B$ the $B$-inner product, and use QR factorization for short to refer to the thin QR factorization (1).

The QR factorization (1) have applications in various numerical algorithms. One application arises from the generalized linear least squares problem

$$\min_x \|Ax - b\|_B. \quad (3)$$

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where $\|v\|_B = \langle v, v \rangle_B^{1/2}$ denotes the $B$-norm. The solution of (3) can be extracted by computing the QR factorization of $A \in \mathbb{R}^{2 \times 10 \times 15}$. Many iterative linear solvers, e.g., the conjugate gradient (CG) method and the preconditioned (generalized) minimal residual (GMRES/MINRES) method, also perform orthogonalization in a non-standard inner product [7, 17], albeit implicitly. When solving Hermitian–definite generalized eigenvalue problems $Ax = Bx\lambda$ or product eigenvalue problems $ABx = x\lambda$ using Krylov subspace methods, where $B$ is positive definite, orthogonalization with the $B$-inner product is often required many times—once in each iteration [4, 5, 15, 23].

When $B = I_k$, there are mainly two classes of algorithms for orthogonalization. One class of algorithms, including Householder–QR [11], Givens–QR [6], and their variants (e.g., TSQR [3]), performs orthogonalization by applying row transformation to the input. We shall call these algorithms row-wise algorithms. Row-wise algorithms eliminate the lower triangular part of $X$ by applying a sequence of unitary operators from the left and eventually transform $X$ to an upper triangular matrix $R$. The unitary operators are then assembled to form the matrix $Q$. The other class of algorithms performs appropriate linear combinations of the columns of $X$ to find an orthonormal basis of $\text{span}(X)$. We shall call this class of algorithms column-wise algorithms. Classical Gram–Schmidt (CGS) and modified Gram–Schmidt (MGS) processes [1, 13] are typical column-wise algorithms. Another frequently used column-wise algorithm is the Cholesky-QR algorithm [5, 24], which first computes the Cholesky factor $R$ of the positive definite matrix $X^HX$ and then solve a triangular system to obtain $Q = XR^{-1}$. When only an orthonormal basis of $\text{span}(X)$ is of interest, the Cholesky factorization of $X^HX$ can be replaced by the spectral decomposition (after proper scaling), leading to the SVQB algorithm [20].

Column-wise algorithms have the advantage that they naturally carry over to the case of non-standard inner products, and, in addition, both Cholesky-QR and SVQB are suitable for high performance computing because they have level 3 arithmetic intensity. However, these algorithms often suffer from numerical instability, and usually require reorthogonalization to improve the orthogonality [13, 24]. Compared to column-wise algorithms, row-wise algorithms have much better numerical stability even if $X$ is rank deficient, because the orthonormal basis is extracted from columns of a (computed) unitary matrix. However, it becomes non-trivial to extend row-wise algorithms to work with a non-standard inner product. We shall see that in the context of a non-standard inner product, a matrix representing a unitary operator usually does not have orthonormal columns.

Recently, Trefethen [21] generalized the method of Householder orthogonalization to the infinite dimensional Hilbert space $L^2[a, b]$. The basic idea is to map a set of vectors to a prescribed orthonormal basis, instead of directly eliminating matrix entries of the input. As long as an orthonormal basis is available, Trefethen’s algorithm can be generalized to work with any separable Hilbert space. Thus it is possible to apply Trefethen’s algorithm to compute the QR factorization [1] with the $B$-inner product. However, by far Trefethen’s algorithm is not considered practical for orthogonalization with the $B$-inner product unless an existing orthonormal basis in the $B$-inner product is already available [14, 12]. We shall discuss how to tackle this issue in practice under mild assumptions.

In this paper we study the computation of (1) based on Householder reflections. We assume that $n \gg k$, and $B$ is not too ill-conditioned so that the $B$-inner product $\langle v, w \rangle_B$ can be evaluated reasonably accurately. These assumptions are valid in many Krylov subspace eigensolvers. We do not require $X$ to have full column rank—$\text{span}(X)$ becomes a proper subspace of $\text{span}(Q)$ if $\text{rank}(X) < k$.

The rest of this paper is organized as follows. In Section 2 we first recall some basic properties of Householder reflections. In Section 3 we present algorithms and variants for Householder orthogonalization with the $B$-inner product. Strategies for constructing an initial orthonormal
basis are discussed in Section\[4\] A brief stability analysis is provided in Section\[5\]. We demonstrate by numerical examples the effectiveness of the proposed algorithms in Section\[6\]. Finally, the paper is concluded in Section\[7\].

2 Householder reflections

In this section we briefly recall some basic properties of Householder reflections.

Let $V$ be a vector space over the field $F$ (for $F \in \{\mathbb{R}, \mathbb{C}\}$) equipped with an inner product $\langle \cdot, \cdot \rangle$. The norm of a vector $x \in V$ is given by $\|x\| = \langle x, x \rangle^{1/2}$. A set of vectors $\{x_1, x_2, \ldots \} \subset V$ is called orthonormal if

$$
\langle x_i, x_j \rangle = \begin{cases} 1 & (i = j), \\ 0 & (i \neq j). 
\end{cases}
$$

Let $w \in V$ be a unit vector, i.e., $\|w\| = 1$. A linear operator $H : V \to V$ defined by

$$
Hx = x - 2w \langle w, x \rangle \quad (\forall x \in V)
$$

is called a Householder reflection or, more precisely, a Householder reflection with respect to the hyperplane orthogonal to $w$. The vector $w$ is known as the Householder vector. It can be easily verified by definition that $H$ is self-adjoint (i.e., $\langle Hx, y \rangle = \langle x, Hy \rangle$ for $x, y \in V$), unitary (i.e., $\langle Hx, Hy \rangle = \langle x, y \rangle$ for $x, y \in V$), and involutory (i.e., $H^2x = x$ for $x \in V$). In addition, for any $x, y \in V$ satisfying $\|x\| = \|y\|$ and $\langle x, y \rangle \in \mathbb{R}$, we can construct a self-adjoint and unitary linear operator of the form $H(\cdot) = I - 2w \langle w, \cdot \rangle$ by choosing

$$
\text{span} \{w\} = \text{span} \{x - y\}, \quad (\|w\| = 1 \text{ or } \|w\| = 0),
$$

such that $Hx = y$ and $Hy = x$. This property plays a key role in the construction of Householder reflections.

When $V = \mathbb{F}^n$ and the inner product is the $B$-inner product induced by a positive definite matrix $B \in \mathbb{F}^{n \times n}$, the situation is slightly more complicated compared to that in an abstract setting, since the canonical basis (i.e., columns of the identity matrix $I_n$) is in general not orthonormal in the $B$-inner product. It is worth noting that there are two different types of orthogonality induced by $B$. The condition $U^HB = I_k$ for $U \in \mathbb{F}^{n \times k}$ means that the columns of $U$ form an orthonormal basis, while the condition $V^HBV = B$ for $V \in \mathbb{F}^{n \times n}$ implies that $V$ is the matrix representation of a unitary operator. These two types of orthogonality are related through

$$
(VU)^HB(VU) = U^H(V^HBV)U = U^HBU = I_k,
$$

which reveals the fact that the unitary operator $V$ maps one orthonormal set $U$ to another orthonormal set $VU$.

A Householder reflection with the $B$-inner product is of the form

$$
H = I_n - 2ww^HB,
$$

where the Householder vector $w$ satisfies $\|w\|_B = 1$. Note that $H^H = H$ does not hold in general when $B \neq I_n$. But a number of properties of Householder reflections in the standard inner product remain valid. For instance, we have $H^2 = I_n$, $H^{-1} = H$, $H^HBH = B$, $\|Hx\|_B = \|x\|_B$, $\det(H) = -1$, and so on. When $\|x\|_B = \|y\|_B \neq 0$, we can find a Householder reflection $H$ such that $y = Hx = H^{-1}x$. In the subsequent section we shall see that the basic idea of Householder orthogonalization is actually using Householder reflections to map a prescribed orthonormal set to the desired one.

\[1\] We allow $w = 0$ in the case $x = y$ to simplify the notation.
3 Householder orthogonalization

In the following we discuss how to make use of Householder reflections to compute the QR factorization \((1)\) in the \(B\)-inner product. Throughout this section we assume that an orthonormal set \(\{u_1, u_2, \ldots, u_k\}\) is available, i.e., we already have a matrix \(U = [u_1, u_2, \ldots, u_k] \in \mathbb{F}^{n \times k}\) such that \(U^HBU = I_k\). Strategies for constructing such a matrix \(U\) will be provided in Section 4.

3.1 Right-looking algorithm

We first discuss a right-looking algorithm for computing the QR factorization. To see how to apply Householder reflections in orthogonalization, we partition \(X\) and \(Q\) into columns, and rewrite \((1)\) as

\[
[x_1, x_2, \ldots, x_k] = [q_1, q_2, \ldots, q_k]
\]

Apply Householder reflections in orthogonalization, we partition \(X\) and \(Q\) into columns, and rewrite \((1)\) as

\[
\begin{bmatrix}
  r_{1,1} & r_{1,2} & \cdots & r_{1,k} \\
  r_{2,1} & r_{2,2} & \cdots & r_{2,k} \\
  \vdots & \vdots & \ddots & \vdots \\
  r_{k,1} & r_{k,2} & \cdots & r_{k,k}
\end{bmatrix}
\]

Let us use the superscript \((1)\) to represent the quantity that is overwritten at the \(i\)th step of the algorithm. Initially, we have \(X = X^{(0)}\). Let \(r_{1,1} = \|x_1^{(0)}\|_B\), and \(v_1 = x_1^{(0)}/r_{1,1}\) if \(r_{1,1} > 0\). A Householder reflection \(H_1 = I_n - 2w_1w_1^H B\) is chosen such that \(H_1u_1 = v_1\), where

\[
w_1 = \frac{v_1 - u_1\alpha_1}{\|v_1 - u_1\alpha_1\|_B}, \quad \alpha_1 = \arg\max_{\alpha \in \mathbb{F}, \|\alpha\| = 1} \|v_1 - u_1\alpha\|_B = -\text{sign}(u_1^HBv_1).
\]

By choosing \(\alpha_1\) in such a way, cancellation can be avoided when computing the Householder vector \(w_1\). In case that \(r_{1,1} = 0\), we simply set \(w_1 = 0\) and there is no need to form \(v_1\) and \(\theta_1\).

The next step is to remove components contributed by \(u_1\) from \(H_1x_2^{(0)}, \ldots, H_1x_k^{(0)}\). This is accomplished by setting

\[
r_{1,i} = u_1^HB(H_1x_i^{(0)}), \quad x_i^{(1)} = H_1x_i^{(0)} - u_1r_{1,i},
\]

for \(i = 2, \ldots, k\). So far we have arrived at

\[
H_1[x_1^{(0)}, x_2^{(0)}, \ldots, x_k^{(0)}] = [u_1r_{1,1}, H_1x_2^{(0)}, \ldots, H_1x_k^{(0)}]
\]

\[
= [u_1, x_2^{(1)}, \ldots, x_k^{(1)}]
\]

\[
\begin{bmatrix}
  r_{1,1} & r_{1,2} & \cdots & r_{1,k} \\
  1 & & & \\
  \vdots & \ddots & \vdots & \vdots \\
  1 & & & 
\end{bmatrix}
\]

A notable property is that \(u_1\) is perpendicular to \(\{x_2^{(1)}, \ldots, x_k^{(1)}\}, u_2, \ldots, u_k\\) in the \(B\)-inner product. By applying the same procedure recursively to \(\{x_2^{(1)}, \ldots, x_k^{(1)}\}\) in the \((n-1)\)-dimensional subspace span \(\{u_1\}^{\perp_B}\) we obtain Householder reflections of the form \(H_i = I_n - 2w_iw_i^HB\) such that

\[
H_k \cdots H_3H_2[x_2^{(1)}, x_3^{(1)}, \ldots, x_k^{(1)}] = [u_2, u_3, \ldots, u_k]
\]

\[
\begin{bmatrix}
  r_{2,2} & r_{2,3} & \cdots & r_{2,k} \\
  r_{3,2} & r_{3,3} & \cdots & r_{3,k} \\
  \vdots & \vdots & \ddots & \vdots \\
  r_{k,2} & r_{k,3} & \cdots & r_{k,k}
\end{bmatrix}
\]

\(^2\)The notation \(\cdot^\perp_B\) denotes the orthogonal complement with the \(B\)-inner product.
When $1 \leq j < i \leq k$, it follows from $u_j^H B w_i = 0$ that
\[ H_i u_j = u_j, \quad (i > j). \tag{8} \]
Therefore, we conclude that
\[ H_k \cdots H_2 H_1 [x_1, x_2, \ldots, x_k] = [u_1, u_2, \ldots, u_k] \begin{bmatrix} r_{1,1} & r_{1,2} & \cdots & r_{1,k} \\ r_{2,1} & r_{2,2} & \cdots & r_{2,k} \\ \vdots & \vdots & \ddots & \vdots \\ r_{k,1} & r_{k,2} & \cdots & r_{k,k} \end{bmatrix} \]
by combining (6) and (7). Let
\[ [q_1, q_2, \ldots, q_k] = H_1 H_2 \cdots H_k [u_1, u_2, \ldots, u_k], \tag{9} \]
or, mathematically equivalently,
\[ q_1 = H_1 u_1, \quad q_2 = H_1 H_2 u_2, \quad \ldots, \quad q_k = H_1 H_2 \cdots H_k u_k, \tag{10} \]
according to (8). It can be easily verified using (4) that $Q^H B Q = I_k$. Thus the QR factorization (5) has been calculated.

We summarize the procedure as Algorithm 1. It is essentially Trefethen’s algorithm, reformulated in a way that we can clearly see from steps (12) that this algorithm is in fact a right-looking algorithm. Step 9 in Algorithm 1 is a reorthogonalization step that mathematically does not change $w_i$’s. However, just like the case for $L^2[a,b]$ as discussed in [21], it is not recommended to skip this step in practice due to the presence of rounding errors, unless certain special structures of $B$ can be exploited to ensure numerical stability. We shall see in Section 6 that skipping such a reorthogonalization step can cause large residual $\|X - QR\|_2$ when $X$ is ill-conditioned. In practice, we observe that the classical Gram–Schmidt process (without further reorthogonalization) is already sufficiently accurate for this step. Finally, we remark that column pivoting can be incorporated in Algorithm 1 so that the diagonal entries of $R$ are decreasing.

### 3.2 Left-looking algorithm

In the following we present a left-looking version of Householder orthogonalization. Albeit being mathematically equivalent to the right-looking algorithm, the left-looking version is suitable in the context of (block) Lanczos/Arnoldi process in which $x_1, \ldots, x_k$ are gradually produced on the fly instead of being immediately available at the beginning.

Let us assume that we have already obtained the QR factorization of $[x_1, \ldots, x_{i-1}]$ as
\[ [x_1, \ldots, x_{i-1}] = H_{i-1} \cdots H_1 [u_1, \ldots, u_{i-1}] R^{(i-1)}, \]
where $R^{(i-1)} \in \mathbb{R}^{(i-1) \times (i-1)}$. Applying one step of classical Gram–Schmidt process on the vector $H_{i-1} \cdots H_1 x_i$ yields
\[ H_{i-1} \cdots H_1 x_i = [u_1, \ldots, u_{i-1}] r_i + v_i \beta_i, \]
where $v_i \in \text{span} \{u_1, \ldots, u_{i-1}\}$ is a unit vector, i.e., $\|v_i\|_B = 1$. Then we construct a Householder reflection $H_i$ satisfying $H_i u_i = v_i$ and $H_i u_j = u_j$ for $1 \leq j < i$ \footnote{For instance, when $B$ is diagonal, $w_i$ is guaranteed to be orthogonal to span $\{u_1, u_2, \ldots, u_{i-1}\}$ both theoretically and numerically. In this case reorthogonalization becomes unnecessary.}. By choosing
\[ R^{(i)} = \begin{bmatrix} R^{(i-1)} & r_i \\ \beta_i & \end{bmatrix} \in \mathbb{R}^{i \times i}, \]
\[ R^{(i)} \begin{bmatrix} r_i \\ \beta_i \end{bmatrix} = \begin{bmatrix} R^{(i-1)} & r_i \\ \beta_i & \end{bmatrix} \]
we obtain the updated QR factorization $[x_1, \ldots, x_{i-1}, x_i] = [u_1, \ldots, u_{i-1}, u_i] R^{(i)}$. Thus the QR factorization (5) has been calculated.

In the following we present a left-looking version of Householder orthogonalization. Albeit being mathematically equivalent to the right-looking algorithm, the left-looking version is suitable in the context of (block) Lanczos/Arnoldi process in which $x_1, \ldots, x_k$ are gradually produced on the fly instead of being immediately available at the beginning.

Let us assume that we have already obtained the QR factorization of $[x_1, \ldots, x_{i-1}]$ as
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where $R^{(i-1)} \in \mathbb{R}^{(i-1) \times (i-1)}$. Applying one step of classical Gram–Schmidt process on the vector $H_{i-1} \cdots H_1 x_i$ yields
\[ H_{i-1} \cdots H_1 x_i = [u_1, \ldots, u_{i-1}] r_i + v_i \beta_i, \]
where $v_i \in \text{span} \{u_1, \ldots, u_{i-1}\}$ is a unit vector, i.e., $\|v_i\|_B = 1$. Then we construct a Householder reflection $H_i$ satisfying $H_i u_i = v_i$ and $H_i u_j = u_j$ for $1 \leq j < i$ \footnote{Similar to the case in the right-looking algorithm, we simply choose $H_i = I_n$ if $\beta_i = 0$.}. By choosing
\[ R^{(i)} = \begin{bmatrix} R^{(i-1)} & r_i \\ \beta_i & \end{bmatrix} \in \mathbb{R}^{i \times i}, \]
which is the QR factorization of

\[ x \]

In the context of a standard inner product, i.e.,

3.3 Compact representation of reflections

admits a compact WY representation of the form

\[ \text{Output: } \text{Matrices } Q \in \mathbb{F}^{n \times k} \text{ and } R \in \mathbb{F}^{k \times k} \text{ satisfying (1) and (2).} \]

for \( i = 1 \text{ to } k \) do

end for

end if

end for

\[ [q_1, \ldots, q_k] \leftarrow [u_1, \ldots, u_k]. \]

for \( i = k \text{ to } 1 \) do

end for

\[ [q_1, \ldots, q_k] \leftarrow [q_i, \ldots, q_k] - 2 w_i u_i^H B[q_i, \ldots, q_n]. \]

end for

we deduce

\[
\begin{bmatrix}
x_1, \ldots, x_{i-1}, x_i
\end{bmatrix}
= H_1 \cdots H_{i-1} [u_1, \ldots, u_{i-1}, H_{i-1}^H \cdots H_1 x_i]
\begin{bmatrix}
R^{(i-1)} & 0 \\
0 & 1
\end{bmatrix}
\]

\[
= H_1 \cdots H_{i-1} [u_1, \ldots, u_{i-1}, u_i] \begin{bmatrix}
R^{(i-1)} & r_i \\
0 & \beta_i
\end{bmatrix}
\]

\[
= H_1 \cdots H_{i-1} H_i [u_1, \ldots, u_{i-1}, u_i] R^{(i)},
\]

which is the QR factorization of \([x_1, \ldots, x_i]\). Repeating this procedure for \( i = 1, 2, \ldots, k \) yields a left-looking algorithm of Householder orthogonalization, as summarized in Algorithm 2. Similar to the right-looking algorithm, a reorthogonalization step using CGS (Step 14) is strongly recommended in finite precision arithmetic.

3.3 Compact representation of reflections

In the context of a standard inner product, i.e., \( B = I_n \), a product of a few Householder reflections admits a compact WY representation of the form

\[
(I - 2 w_1 u_1^H) \cdots (I - 2 w_k u_k^H) = I_n + WTW^H,
\]

where \( W \in \mathbb{F}^{n \times k} \) is lower trapezoidal and \( T \in \mathbb{F}^{k \times k} \) is upper triangular [19]. The compact WY representation is important for high performance computing since it provides opportunities for efficient applications of a sequence of Householder reflections using level 3 BLAS. By relaxing the requirement on the nonzero pattern of \( W \), the compact WY representation easily carries over to Householder reflections with a non-standard inner product.
Algorithm 2 Left-looking Householder orthogonalization algorithm

Input: A matrix $X \in \mathbb{F}^{n \times k}$ to be orthogonalized, a positive definite matrix $B \in \mathbb{F}^{n \times n}$, and $U \in \mathbb{F}^{n \times k}$ such that $U^HBU = I_k$.

Output: Matrices $Q \in \mathbb{F}^{n \times k}$ and $R \in \mathbb{F}^{k \times k}$ satisfying \([1]\) and \([2]\).

1: for $i = 1$ to $k$ do
2:   for $j = 1$ to $i - 1$ do
3:     $x_i \leftarrow x_i - 2w_jw_j^HBx_i$.
4:   end for
5:   $[r_{1,i}, \ldots, r_{i-1,i}]^T \leftarrow [u_1, \ldots, u_{i-1}]^H Bx_i$.
6:   $x_i \leftarrow x_i - [u_1, \ldots, u_{i-1}][r_{1,i}, \ldots, r_{i-1,i}]^T$.
7:   $r_{i,i} \leftarrow \|x_i\|_B$.
8:   if $r_{i,i} = 0$ then
9:     $w_i \leftarrow 0$.
10: else
11:   $x_i \leftarrow x_i/r_{i,i}$.
12:   $u_i \leftarrow \text{sign}(u_i^H Bx_i)u_i$.
13:   $w_i \leftarrow x_i - u_i$.
14:   (optional) $w_i \leftarrow w_i - [u_1, \ldots, u_{i-1}][u_1, \ldots, u_{i-1}]^H Bw_i$.
15:   $w_i \leftarrow w_i/\|w_i\|_B$.
16: end if
17: end for
18: $[q_1, \ldots, q_k] \leftarrow [u_1, \ldots, u_k]$.
19: for $i = k$ to $1$ do
20:   $[q_i, \ldots, q_k] \leftarrow [q_i, \ldots, q_k] - 2w_iw_i^HB[q_i, \ldots, q_k]$.
21: end for

Let $W_i = [w_i, w_2, \ldots, w_i]$ for $i \leq k$, and $H_i = I_n - 2w_iw_i^HB$ be Householder reflections (with $W_k^H B W_k = I_k$). Suppose that we already have a compact WY representation of the form

$$H_1 \cdots H_{i-1} = I_n - 2W_{i-1}T_{i-1}W_{i-1}^HB,$$

where $T_{i-1} \in \mathbb{F}^{(i-1) \times (i-1)}$ is unit upper triangular. Then it can be verified that

$$H_1 \cdots H_{i-1}H_i = I_n - 2W_iT_iW_i^HB,$$  \hspace{1cm} (12)

where

$$T_i = \begin{bmatrix} T_{i-1} & 2T_{i-1}W_{i-1}^HBw_i \\ 1 & \end{bmatrix} \in \mathbb{F}^{i \times i}$$

is also unit upper triangular.

The compact WY representation \([12]\) generalizes \([11]\), despite that a slightly different scaling convention is adopted here. Some care needs to be taken when we need to apply the transformations in reversed order. Since the matrix $H_1 \cdots H_k$ in \([12]\) is not unitary (in the standard inner product), we cannot invert the right-hand side of \([12]\) by directly taking the conjugate transpose. Instead, we have

$$H_k \cdots H_1 = (H_1 \cdots H_k)^{-1} = I_n - 2W_kT_kW_k^HB,$$  \hspace{1cm} (13)

which is essentially the adjoint operator of $H_1 \cdots H_k$ in the $B$-inner product.

The compact WY representation of Householder reflections is useful in Householder orthogonalization, especially when $k$ is not so small. Even for a small $k$ we can still make use of the
compact WY representation in the left-looking algorithm. For instance, \[ \mathbf{U} \] can be used to compute \( H_1 H_2 \cdots H_k \) in Algorithm 2 (steps 2-4). When \( k \) is of medium size (e.g., \( k = O(1000) \), which is typical in electronic structure calculations [4]), we may design a block algorithm that mixes Algorithms 1 and 2. Partition \( X \) into a few \( n \times b \) panels, where \( 1 \ll b \ll k \); use the left-looking algorithm for panel factorization, and then apply a block version of the right-looking algorithm to update the remaining columns of \( X \). In such a block algorithm, arithmetic intensity can be improved by making use of the WY representation in the right-looking update. We remark that, if implemented carefully, the compact WY representation can also be adopted in the final steps of Algorithms 1 and 2 i.e., computing

\[
[q_1, q_2, \ldots, q_k] = H_1 H_2 \cdots H_k [u_1, u_2, \ldots, u_k].
\]

A naive application of (12) without taking into account (8) roughly doubles the computational cost, and increases rounding errors. Hence a block approach is more appropriate when \( k \) of modest size. However, detailed discussions concerning high performance computing aspects is beyond the scope of this paper.

4 Construction of an initial orthonormal basis

In the previous section, we assume that a matrix \( U \in \mathbb{F}^{n \times k} \) satisfying \( U^H BU = I_k \) is already available. The algorithms heavily relies on the availability of \( U \). In Trefethen’s original work [21], the set of scaled Legendre polynomials is naturally available as an orthonormal basis of \( L^2[a, b] \). However, in general an obvious choice does not exist for \( F^n \) with the \( B \)-inner product. In this section we discuss how to construct an initial orthonormal basis in practice.

When \( k \) is close to \( n \), finding a matrix \( U \) with \( U^H BU = I_k \) is not much cheaper than computing the Cholesky factorization of \( B \) unless certain special structures of \( B \) can be exploited. This is the main obstacle for Householder orthogonalization in a very generic setting. However, we are mainly interested in the case \( k \ll n \), which is the typical situation in practice. In this case there is no need to find an entire orthonormal basis of \( \mathbb{F}^n \). Instead, an orthonormal basis of any \( k \)-dimensional subspace suffices.

Let \( \tilde{B} \) be the leading \( k \times k \) principal submatrix of \( B \). Then \( \tilde{B} \) is positive definite, and admits a Cholesky factorization \( \tilde{B} = \tilde{R}^T \tilde{R} \). It can be easily verified that

\[
U = \begin{bmatrix} \tilde{R}^{-1} & 0 \\ \end{bmatrix} \in \mathbb{F}^{n \times k}
\]

satisfies \( U^H BU = \tilde{R}^{-H} \tilde{B} \tilde{R}^{-1} = I_k \). If the matrix \( B \) is explicitly stored, constructing \( U \) requires as cheap as \( O(k^3) \) operations and \( O(k^2) \) storage. This cost is negligible, since any practical orthogonalization algorithm requires \( O(nk^2) \) dense linear algebra operations in addition to \( O(k) \) matrix–vector multiplications. Even if the matrix \( B \) is only implicitly available through a black box function \( x \mapsto Bx \), we have \( \tilde{B} = E_k^H B E_k \), where \( E_k = [e_1, e_2, \ldots, e_k] \) denotes the leading columns of the identity matrix \( I_n \). The cost consists of \( O(k^3) \) dense operations and \( O(k) \) matrix–vector multiplications, which is still lower than the entire orthogonalization algorithm. Therefore, we have obtained a strategy, as summarized in Algorithm 3, to construct \( U \) with affordable overhead.

Algorithm 3 can be viewed as the Cholesky-QR algorithm applied to \( E_k \). The idea is similar to that of the PRECHOL-QR algorithm in [13]. Unlike the general Cholesky-QR algorithm which is very sensitive to rounding errors, we use a well-conditioned input with \( \kappa_2(E_k) = 1 \) and

\[
\kappa_2(A) = \|A\|_2 \|A^\dagger\|_2
\]

represents the condition number of \( A \), where \( A^\dagger \) is the Moore–Penrose pseudoinverse of \( A \).
Algorithm 3 Construction of an initial orthonormal set

**Input:** A positive definite matrix $B \in \mathbb{R}^{n \times n}$, a positive integer $k \leq n$.

**Output:** A matrix $U \in \mathbb{R}^{n \times k}$ such that $U^HBU = I_k$.

1. $\tilde{B} \leftarrow$ the $k \times k$ leading submatrix of $B$.
2. Compute the Cholesky factorization $\tilde{B} = \tilde{R}^H\tilde{R}$.
3. $U \leftarrow [\tilde{R}^{-H}, 0]^H$.

the Gramian matrix $\tilde{B}$ is often reasonably well-conditioned. Theoretically, it follows from the Cauchy interlacing theorem that $\kappa_2(\tilde{B}) \leq \kappa_2(B)$. Though the extreme case $\kappa_2(\tilde{B}) = \kappa_2(B)$ may occur, very often we can even expect $\kappa_2(\tilde{B}) \ll \kappa_2(B)$ in practice as long as $k$ is not too large.

Certainly there exist many alternatives to Algorithm 3. For instance, choosing any columns from the identity matrix works equally well. Besides the canonical basis with the standard inner product, other well-conditioned basis can also be used to construct $U$, as long as the Gramian matrix is not too ill-conditioned. The freedom of replacing $E_k$ by other matrices comes at a price of possibly higher rounding errors. In the case that $\tilde{B}$ is ill-conditioned, some iterative refinement strategies (e.g., shifted Cholesky-QR [5], possibly using extended precision arithmetic [25]) can be adopted to improve the orthogonality of $U$.

In the context of Krylov subspace methods that perform orthogonalization in each iteration, there are alternative strategies for constructing $U$. For instance, we may use another orthogonalization algorithm (e.g., modified Gram–Schmidt process with reorthogonalization) in the first iteration to obtain an orthonormal basis, and then use this basis as $U$ in the subsequent iterations. Algorithm 3 also becomes more appealing compared to the case that only one set of vectors needs to be orthogonalized, since $U$ is constructed only once and then can be reused many times. Hence, the overhead for constructing $U$ becomes negligible in this setting, even by taking into account the cost of optional iterative refinement with extended precision arithmetic.

5 Numerical orthogonality

In the following we discuss the numerical orthogonality of Householder reflections with the $B$-inner product in finite precision arithmetic. We shall show that under mild assumptions the computed Householder reflections are orthogonal.

5.1 Rounding models

On most modern computational units, if there is no overflow or (gradual) underflow in the calculation, we can assume that the computed results for finite numbers, denoted by fl(·)’s, satisfy

$$
fl(a \circ b) = (a \circ b)(1 + \epsilon_1), \quad fl(c^{1/2}) = c^{1/2}(1 + \epsilon_2),
$$

for $a, b \in \mathbb{F}$, $\circ \in \{+, -, \times, /\}$, $(b, \circ) \neq (0, /)$, and $c \in [0, +\infty)$, where the machine precision $u$ is an upper bound of max $\{|\epsilon_1|, |\epsilon_2|\}$. The rounding model [14] is valid for both real and complex arithmetic since $u_{\text{complex}}$ is a small multiple of $u_{\text{real}}$ [9, Section 3.6].

Unlike existing rounding error analysis directly based on [13] as in [14] [16] [24], we provide a higher level abstraction that illustrates major sources of rounding errors. We first assume that the $B$-inner product is evaluated in a backward stable manner in the sense that

$$
fl(v^HBw) = v^H(B + \Delta B)w, \quad \|\Delta B\|_2 \leq \epsilon_B\|B\|_2,
$$

(15)
where $\epsilon_B \geq \mathbf{u}$ is a constant. In fact, if $v \neq 0$ and $w \neq 0$, a rank-one backward error can be chosen as

$$\Delta B = \frac{\|v^H B w - v^H B w\|}{\|v\|_2 \|w\|_2} \cdot \frac{v u^H}{\|v\|_2 \|w\|_2}.$$ 

The model [15] is plausible because it merely requires a weak assumption that

$$\sup_{v, w \neq 0} \frac{\|v^H B w - v^H B w\|}{\|B\|_2 \|v\|_2 \|w\|_2} < +\infty.$$ 

Based on the model [15], we conclude that evaluating the $B$ -norm of a nonzero vector $w$ introduces a relative error bounded by $\kappa_2(B)\epsilon_B$ because

$$\frac{\|v^H B w - v^H B w\|}{w^H B w} = \frac{\|w^H \Delta B w\|}{w^H B w} \leq \|B^{-1/2} \Delta B B^{-1/2}\|_2 \leq \kappa_2(B)\epsilon_B.$$ 

Therefore, we make another assumption that normalizing a vector with the $B$-norm in finite precision arithmetic introduces an error no more than $\epsilon_n$. To be more precise, the normalization operation $\tilde{w} = w/(w^H B w)^{1/2}$ produces an approximate unit vector $\tilde{w}$ that satisfies

$$\|\tilde{w}\|_B^2 = \tilde{w}^H B \tilde{w} = 1 + \epsilon, \quad |\epsilon| \leq \epsilon_n,$$ 

(16)

where $\epsilon_n$ represents the normalization error bound. When $B$ is numerically positive definite, we can assume $\kappa_2(B)\epsilon_B < 1$. Then there exists

$$\epsilon_n \leq \frac{1}{1 - \kappa_2(B)\epsilon_B} - 1 = \frac{\kappa_2(B)\epsilon_B}{1 - \kappa_2(B)\epsilon_B} = O(\kappa_2(B)\epsilon_B).$$

Though $\epsilon_B$ and $\epsilon_n$ are closely related, instead of bounding all errors in terms of $\epsilon_B$, we shall make use of $\epsilon_n$ whenever possible. Normalization errors are ubiquitous in all orthogonalization algorithms (including Gram–Schmidt processes, Cholesky-QR, SVQ2, as well as Householder-QR) that involve the evaluation of $B$-inner products. In the extreme case, even normalizing a perfectly orthogonal set of vectors introduces normalization errors. A necessary condition for any orthogonalization algorithm to proceed without breakdown is $\epsilon_n < 1$, i.e., $B$ at least needs to be numerically positive definite. It can be expected that $\epsilon_n$ plays an important role in characterizing the numerical orthogonality.

While in general we expect $\epsilon_B = O(\mathbf{u})$ and $\epsilon_n = O(\kappa_2(B)\mathbf{u})$, the concrete values of $\epsilon_B$ and $\epsilon_n$ depend on how accurately the matrix–vector multiplication $w \mapsto Bw$ is performed. Using $\epsilon_B$ and $\epsilon_n$ treats the operation $w \mapsto Bw$ as a black box, while still allows algorithmic details of matrix–vector multiplication to be taken into account. For instance, if the entries of $B$ are explicitly available and $2n\mathbf{u} < 1$, it can be shown (see, e.g., [9] Section 3)) that

$$|\Delta B| \leq \frac{2n\mathbf{u}}{1 - 2n\mathbf{u}} |B|^6$$

and hence

$$\frac{\|\Delta B\|_2}{\|B\|_2} \leq \frac{2n\mathbf{u}}{1 - 2n\mathbf{u}} \cdot \frac{\|B\|_2}{\|B\|_2} \leq \frac{2n\mathbf{u}}{1 - 2n\mathbf{u}} \cdot \frac{n^{-1/2} \|B\|_F}{n^{-1/2} |B|_F} = \frac{2n^{3/2} \mathbf{u}}{1 - 2n\mathbf{u}}.$$ 

It is then possible to substitute $\epsilon_B$ by the corresponding upper bound. Alternative estimates of $\epsilon_B$ and $\epsilon_n$, whenever available, are also applicable.

---

Both the notation of absolute value and the inequality are understood entrywise.
5.2 Orthogonality of computed Householder reflections

A computed Householder reflection \( \hat{H}_t = I_n - 2\hat{w}_i\hat{w}_i^H B \) is represented by the corresponding Householder vector \( \hat{w}_i \). By our assumption, \( \hat{w}_i \) satisfies \( |\hat{w}_i^H B \hat{w}_i - 1| \leq \epsilon_n \). We first establish a structured backward error estimate regarding the orthogonality of Householder reflections as shown in Lemma 1.

**Lemma 1.** Let \( \hat{H} = \hat{H}_1 \hat{H}_2 \cdots \hat{H}_k \) with \( \hat{H}_i = I_n - 2\hat{w}_i\hat{w}_i^H B \) satisfying \( |\hat{w}_i^H B \hat{w}_i - 1| \leq \epsilon_n \) for \( i = 1, 2, \ldots, k \), where \( B \in \mathbb{C}^{n \times n} \) is a positive definite matrix. Then there exists a Hermitian matrix \( \Delta_k \in \mathbb{R}^{n \times n} \) such that

\[
\hat{H}^H B \hat{H} = B^{1/2} (I_n + \Delta_k) B^{1/2}
\]

and

\[
\|\Delta_k\|_2 \leq 4k\epsilon_n(1 + \epsilon_n)^{4k-2}.
\]

**Proof.** We prove this lemma by induction. For \( k = 1 \), we have

\[
\hat{H}_1^H B \hat{H}_1 = B + 4B\hat{w}_1(\hat{w}_1^H B \hat{w}_1 - 1)\hat{w}_1^H B
\]

\[
= B^{1/2} (I_n + 4\hat{z}_1(\hat{z}_1^H \hat{z}_1 - 1)\hat{z}_1^H) B^{1/2},
\]

where \( \hat{z}_1 = B^{1/2} \hat{w}_1 \). Let \( \Delta_1 = 4\hat{z}_1(\hat{z}_1^H \hat{z}_1 - 1)\hat{z}_1^H \). Then

\[
\|\Delta_1\|_2 = 4\|\hat{z}_1\|^2 |\hat{z}_1^H \hat{z}_1 - 1| \leq 4\epsilon_n(1 + \epsilon_n)^2.
\]

For \( k > 1 \), we have

\[
(\hat{H}_1 \hat{H}_2 \cdots \hat{H}_k)^H B (\hat{H}_1 \hat{H}_2 \cdots \hat{H}_k) = \hat{H}_k^H B \hat{H}_k + \hat{H}_k^H B^{1/2} \Delta_{k-1} B^{1/2} \hat{H}_k
\]

\[
= \hat{H}_k^H B \hat{H}_k + B^{1/2} (I_n - 2\hat{z}_k \hat{z}_k^H) \Delta_{k-1} (I_n - 2\hat{z}_k \hat{z}_k^H) B^{1/2},
\]

where \( \hat{z}_k = B^{1/2} \hat{w}_k \). Let

\[
\Delta_k = 4\hat{z}_k(\hat{z}_k^H \hat{z}_k - 1)\hat{z}_k^H + (I_n - 2\hat{z}_k \hat{z}_k^H) \Delta_{k-1} (I_n - 2\hat{z}_k \hat{z}_k^H).
\]

It can be verified that

\[
\|I_n - 2\hat{z}_k \hat{z}_k^H\|_2 = \max \{1, |1 - 2\hat{z}_k \hat{z}_k^H|\} \leq 1 + 2\epsilon_n.
\]

Then it follows from the inductive hypothesis that

\[
\|\Delta_k\|_2 \leq 4\|\hat{z}_k^H (\hat{z}_k^H \hat{z}_k - 1)\hat{z}_k^H\|_2 + \|I_n - 2\hat{z}_k \hat{z}_k^H\|^2 \|\Delta_{k-1}\|_2
\]

\[
\leq 4\epsilon_n(1 + \epsilon_n)^2 + (1 + 2\epsilon_n)^2 \cdot 4(1 - \epsilon_n(1 + \epsilon_n))^{4k-6} - 6
\]

\[
\leq 4\epsilon_n(1 + \epsilon_n)^2 + 4(1 - \epsilon_n(1 + \epsilon_n))^{4k-2} - 6
\]

\[
\leq 4k\epsilon_n(1 + \epsilon_n)^{4k-2}.
\]

By Lemma 1, we deduce

\[
\frac{\|\hat{H}^H B \hat{H} - B\|_2}{\|B\|_2} = \frac{\|B^{1/2} \Delta_k B^{1/2}\|_2}{\|B\|_2} \leq \frac{\|\Delta_k\|_2 \|B^{1/2}\|_2^2}{\|B\|_2} \leq 4k\epsilon_n(1 + \epsilon_n)^{4k-2}
\]

for \( \hat{H} = \hat{H}_1 \hat{H}_2 \cdots \hat{H}_k \). This result is stated as Theorem 2 below.
**Theorem 2.** Under the same assumption of Lemma 1 we have
\[
\frac{\|\hat{H}^H B \hat{H} - B\|_2}{\|B\|_2} \leq 4k\epsilon_n(1 + \epsilon_n)^{4k-2}.
\]

The upper bound in Theorem 2 is satisfactory in the sense that it is a small multiple of \(\epsilon_n\), and, roughly speaking, grows merely linearly with \(k\). For instance, if \((4k - 2)\epsilon_n \leq 1/2\), which can be achieved for reasonably well-conditioned \(B\)’s, we have
\[
\frac{\|\hat{H}^H B \hat{H} - B\|_2}{\|B\|_2} \leq 4k\epsilon_n(1 + \epsilon_n)^{4k-2} \leq \frac{4k\epsilon_n}{1 - (4k - 2)\epsilon_n} \leq 8k\epsilon_n = O(\epsilon_n).
\]

In the case that \(\epsilon_n\) far overestimates the normalization error for the given set of Householder vectors, \(\epsilon_n\) can be replaced by \(\max_{1 \leq i \leq k}\|\hat{w}_i^H B \hat{w}_i - 1\|\) for a tighter estimate. It is worth noting that the error estimate does not depend on the magnitude of each \(\|w_i - \hat{w}_i\|_2\). Even span \{\hat{w}_i\}’s are really far away from span \{\hat{w}_i\}’s, \(\hat{H}\) is still close to orthogonal if \(\hat{w}_i\)’s are properly normalized. Only the normalization errors in \(\hat{w}_i\)’s play a role.

### 5.3 Orthogonality of computed orthonormal basis

Theorem 2 illustrates the loss of orthogonality for \(\hat{H}\) as an approximate unitary operator. We are also interested in the numerical orthogonality of \(\hat{H}\hat{U}\) in the QR factorization, where \(\hat{U}\) is the (approximate) initial orthonormal basis. The loss of orthogonality for \(\hat{H}\hat{U}\) is provided in Theorem 3.

**Theorem 3.** Under the same assumption of Lemma 1 for any \(\hat{U} \in \mathbb{R}^{n \times k}\) we have
\[
\|(\hat{H}\hat{U})^H B(\hat{H}\hat{U}) - I_k\|_2 \leq \epsilon_0 + 4k\epsilon_n(1 + \epsilon_0)(1 + \epsilon_n)^{4k-2},
\]
where
\[
\epsilon_0 = \|\hat{U}^H B \hat{U} - I_k\|_2.
\]

**Proof.** Using Lemma 1 we have
\[
\|(\hat{H}\hat{U})^H B(\hat{H}\hat{U}) - I_k\|_2 \leq \|(\hat{H}\hat{U})^H B(\hat{H}\hat{U}) - (\hat{H}\hat{U})\|_2 + \|(\hat{H}\hat{U})^H B \hat{H} - B)\hat{U}\|_2
\]
\[
= \epsilon_0 + \|\hat{U}^H B^1/2 \Delta_k B^{1/2} \hat{U}\|_2
\]
\[
\leq \epsilon_0 + \|B^{1/2} \hat{U}\|_2 \|\Delta_k\|_2
\]
\[
= \epsilon_0 + \|\hat{U}^H B \hat{U}\|_2 \|\Delta_k\|_2
\]
\[
\leq \epsilon_0 + 4k\epsilon_n(1 + \epsilon_0)(1 + \epsilon_n)^{4k-2}.
\]

The error bound in Theorem 3 can be roughly understood as \(O(\epsilon_0 + k\epsilon_n)\). We see that there are two sources of errors—the initial orthogonalization error \(\epsilon_0\) contributed by \(\hat{U}\), and a small multiple of \(\epsilon_n\) contributed by \(\hat{H}\). If \(\hat{U}\) is constructed by Algorithm 3, it can be shown (see, e.g., Chapter 14) that \(\epsilon_0 \leq O(k^3)\epsilon_2(B)u\). When \(\epsilon_0\) is too large, it is recommended to refine \(\hat{U}\) using, e.g., extended precision.

When \(Q = \hat{H}\hat{U}\) needs to be explicitly formed, there is an additional source of rounding errors characterized in the following Theorem 4. Its proof is a bit lengthy, and can be found in the Appendix. We remark that in the proof of Theorem 4 concretes estimate of the prefactor in the big-\(O\) notation is not very important since we are mainly interested in the asymptotic behavior of numerical orthogonality. Nevertheless, omitting this prefactor does not cause an abuse of the big-\(O\) notation.
n = 2000; k = 100;
logkappaB = 5;
Q = orth(randn(n) + 1i*randn(n));
U = orth(randn(n, k) + 1i*randn(n, k));
V = orth(randn(k) + 1i*randn(k));
B = Q* diag (logspace (0 , -logkappaB , n ))*Q'; B = (B + B')/2;
for logkappaX = 0:16 ,
X = U* diag (logspace (0 , -logkappaX , n ))* V;
...
end

Figure 1: Code snippet for generating random test matrices with prescribed condition numbers.

**Theorem 4.** Let \( \hat{U} \in F^{n \times k} \) whose columns are normalized according to \( \{16\} \), and \( \hat{Q} = \Pi(\hat{U}) \).
Under the assumption of Lemma \( \{7\} \) and \( 18k\kappa_2(B)\epsilon_B < 1 \), we have
\[
\| \hat{Q}^H B \hat{Q} - I_k \|_2 = \epsilon_o + O(k^2 \kappa_2(B)\epsilon_B),
\]
where \( \epsilon_o = \| \hat{U}^H B \hat{U} - I_k \|_2 \leq 1 \).

In summary, our stability analysis suggests that Householder reflections have nice numerical orthogonality under mild assumptions over \( B \). In order to attain good orthogonality in practice, it is important to ensure the orthogonality of the initial orthonormal basis \( \hat{U} \), and try to evaluate the \( B \)-inner product as accurately as possible.

It can be seen from the theoretical results that the numerical orthogonality of Householder reflections may depend on \( \kappa_2(B) \), while does not depend on \( \kappa_2(X) \). In fact, the analysis is valid for Householder reflections computed from any source, not necessarily from orthogonalizing \( X \). Therefore, \( \kappa_2(X) \) does not play any role here.

6 Numerical experiments

In the following we present numerical results for our Householder orthogonalization algorithms. Algorithm \( \{3\} \) is used for constructing the initial orthonormal basis. Test results for classical and modified Gram–Schmidt processes, with and without reorthogonalization, are also provided for comparison. All experiments are performed on a GNU Linux computer running Debian version 10 (buster) using GNU Octave version 4.4.1 (configured for x86_64-pc-linux-gnu) under double-precision arithmetic, where the machine precision (for real numbers) is \( u = 2^{-53} \approx 1.1 \times 10^{-16} \).

6.1 Random test matrices

We first generate a reasonably well-conditioned Hermitian positive definite matrix \( B \in \mathbb{C}^{2000 \times 2000} \) with \( \kappa_2(B) = 10^5 \), and test it with a few different \( X \)’s in \( \mathbb{C}^{2000 \times 100} \) by varying \( \kappa_2(X) \in [10^6, 10^{16}] \). The code snippet for generating random test matrices with prescribed condition numbers is shown in Figure \( \{1\} \).

Figures \( 2(a) \) and \( 2(b) \) show the losses of orthogonality and the relative residuals, respectively. Without reorthogonalization, neither CGS nor MGS retains numerical orthogonality as \( \kappa_2(X) \) grows\(^7\). CGS2, MGS2, and both variants of Householder orthogonalization are numerically

\(^7\)CGS2 and MGS2, respectively, represent variants of CGS and MGS with reorthogonalization.
stable, regardless of the magnitude of $\kappa_2(X)$. The accuracy of Householder orthogonalization is satisfactory, though being slightly lower compared to that of CGS2 and MGS2.

We then repeat the same set of tests on another randomly generated ill-conditioned matrix $B$ with $\kappa_2(B) = 10^{15}$. The test results are shown in Figures 2(c) and 2(d). All algorithms behave similarly compared to the previous test. The numerical stability of Householder orthogonalization is again satisfactory, and is independent of the conditioning of $X$.

As suggested in Section 3, in practice a step of reorthogonalization (Step 9 in Algorithm 1 and Step 14 in Algorithm 2) is strongly recommended for numerical stability. Figure 3 shows the consequence if such a reorthogonalization step is skipped. We compare two variants for accumulating the Householder reflections—(9) and (10)—depending on whether (8) is used. The corresponding variants are labeled as ‘full’ and ‘half’, respectively, in Figure 3. By skipping the reorthogonalization step, the use of (10) causes loss of orthogonality and/or large residual when $X$ becomes increasingly ill-conditioned. However, when (9) is adopted, with the price of almost double computational cost compared to (10), the numerical orthogonality of $Q$ is retained though the residual still increases as $\kappa_2(X)$ increases. This is consistent with the theoretical analysis in Section 5—accumulated Householder reflections are numerically orthogonal as long as the Householder vectors are accurately normalized. Interestingly, Figure 3 suggests that
Figure 3: Losses of orthogonality (left) and relative residual (right) for different variants of Householder orthogonalization. ‘(R)’ and ‘(L)’, respectively, stand for right-looking and left-looking algorithms. Labels ‘full’ and ‘half’ are used to denote strategies (9) and (10), respectively, for accumulating the Householder reflections. The label ‘reorth’ stands for the ‘correct’ implementation of Algorithms 1 and 2, both based on (10).

sometimes an accuracy of $O(u^{1/2})$ can be achieved even for very ill-conditioned $X$’s. A careful rounding error analysis will be needed in order to explain this behavior.

6.2 A rank deficient example

To illustrate the robustness of Householder orthogonalization, we use an extremely ill-conditioned test case constructed as follows. The matrices $B \in \mathbb{C}^{2000 \times 2000}$ and $X_0 \in \mathbb{C}^{2000 \times 10}$ are generated using the technique shown in Figure 2 such that $\kappa_2(B) = \kappa_2(X_0) = 10^{20}$. Numerically, GNU Octave reports $\text{cond}(B) \approx 5.9 \times 10^{19}$ and $\text{cond}(X_0) \approx 2.5 \times 10^{16}$. Then we choose $X$ as

$$X = [X_0, 0 \cdot X_0, X_0] \in \mathbb{C}^{2000 \times 30},$$

which is rank deficient, and compute the QR factorization of $X$. This problem is challenging since both $B$ and $X$ are extremely ill-conditioned.

Table 1 shows the losses of orthogonality and relative residuals for this problem. Since $X$ is rank deficient and contains zero columns, Gram–Schmidt processes are implemented in a way

$$\|X - QR\|_2/\|X\|_2 = \kappa_2(B) = 10^{15}$$

$$\kappa_2(B) = 10^{15}$$

$$\kappa_2(B) = 10^{5}$$

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Table 1: Losses of orthogonality and relative residuals for the rank deficient test problem \((17)\). The column “rank\((Q)\)” reports the number of vectors in the orthonormal basis computed by each method.

| Method       | rank\((Q)\) | \(\|Q^H B Q - I\|_2\) | \(\|X - QR\|_2 / \|X\|_2\) |
|--------------|-------------|----------------|-----------------|
| CGS          | 20          | \(1.5 \times 10^4\) | \(5.7 \times 10^{-6}\) |
| MGS          | 20          | \(1.5 \times 10^0\)  | \(6.7 \times 10^{-17}\) |
| CGS2         | 20          | \(5.0 \times 10^0\)  | \(2.5 \times 10^0\)   |
| MGS2         | 20          | \(1.0 \times 10^0\)  | \(6.1 \times 10^{-17}\) |
| Householder (R) | 30        | \(6.5 \times 10^{-15}\) | \(1.0 \times 10^{-15}\) |
| Householder (L) | 30        | \(4.5 \times 10^{-15}\) | \(1.7 \times 10^{-15}\) |

that a column \(\hat{q}_i\) is dropped when numerically encountering \(\hat{q}_i^H B \hat{q}_i \leq 0\) during normalization. Then all variants of Gram–Schmidt processes produce 20 vectors, while none of these bases has satisfactory orthogonality. CGS and CGS2 even yield large residuals. However, both variants of Householder orthogonalization still work well for this challenging problem. Though the matrix \(B\) is extremely ill-conditioned, its \(30 \times 30\) leading principal submatrix \(\tilde{B}\) is well-conditioned (in fact, GNU Octave reports \(\kappa_2(\tilde{B}) \approx 7.8\)). As a result, Algorithm 3 successfully produces a very good initial orthonormal basis for this problem. Then Householder orthogonalization produces an orthonormal basis for a 30-dimensional subspace, and achieves small factorization error.

### 6.3 Examples with numerical difficulties

Previous examples illustrate that in practice the (worst-case) rounding analysis may be too pessimistic. Numerical stability can sometimes be expected even for ill-conditioned matrices. However, even though rounding errors may be severely overestimated for concrete examples, the theoretical analysis still suggests potential sources of numerical difficulties.

In order to construct examples such that the matrix–vector multiplication \(x \mapsto Bx\) has relatively large rounding errors, we choose \(\text{span}(X)\) to be the invariant subspace spanned by eigenvectors corresponding to the five smallest eigenvalues of \(B\), where \(B \in \mathbb{C}^{2000 \times 2000}\) is randomly generated with prescribed condition numbers as shown in Figure 1. The eigenvectors are rotated by a random \(5 \times 5\) unitary matrix to form the columns of \(X\). Figures 4(a) and 4(b) show the losses of orthogonality and the relative residuals, respectively, when varying \(\kappa_2(B)\). The loss of orthogonality grows linearly with respect to \(\kappa_2(B)\) as predicted by Theorem 4. We repeat the same experiment by choosing \(\text{span}(X)\) to be the invariant subspace spanned by eigenvectors corresponding to the five largest eigenvalues of \(B\). The results are shown in Figures 4(c) and 4(d). The loss of orthogonality in this case remains low as \(\kappa_2(B)\) varies, likely because the actual normalization error is much lower than \(\epsilon_n\). These experiments also suggest that the bound on relative residuals may also depend linearly with \(\kappa_2(B)\). More insight into the computed residual norms is planned as our future work.

Finally, we show that Householder orthogonalization can sometimes fail, in the sense that the outputs are not accurate at all. Let us use the matrix \(B\) from Section 6.2, while \(X\) is chosen to be the eigenvectors corresponding to the five smallest eigenvalues of \(B\) and normalized in the standard inner product. Theoretically, \(X\) is perfectly conditioned, and even columns of \(X\) are already orthogonal in the \(B\)-inner product. However, since \(B\) is too ill-conditioned, the normalization error bound \(\epsilon_n\) is expected to be greater than one in this case. Table 2 shows the losses of orthogonality and relative residuals obtained by different methods. The numerical orthogonality is lost for all methods due to large normalization errors. This agrees
Figure 4: Losses of orthogonality (left) and relative residual (right) for Householder orthogonalization by varying $\kappa_2(B)$. 'R' and 'L', respectively, stand for right-looking and left-looking algorithms. Labels 'bottom' and 'top', respectively, imply that $X$ is constructed from the invariant subspaces corresponding to the bottom and top ends of the spectrum of $B$.

Table 2: Losses of orthogonality and relative residuals for $X$ consisting eigenvectors corresponding to the smallest eigenvalues of an ill-conditioned $B$.

| Method            | $\|Q^TBQ - I\|_2$ | $\|X - QR\|_2/\|X\|_2$ |
|-------------------|--------------------|-------------------------|
| CGS               | $5.5 \times 10^0$  | $1.5 \times 10^{-15}$   |
| MGS               | $6.3 \times 10^0$  | $2.0 \times 10^{-15}$   |
| CGS2              | $7.8 \times 10^0$  | $4.0 \times 10^{-15}$   |
| MGS2              | $1.0 \times 10^0$  | $2.5 \times 10^{-15}$   |
| Householder (R)   | $2.6 \times 10^2$  | $1.1 \times 10^2$       |
| Householder (L)   | $2.4 \times 10^4$  | $2.4 \times 10^4$       |

with the prediction by the theoretical analysis. Householder orthogonalization even produces large residuals here.
7 Concluding remarks

In this paper we have discussed how to compute a tall-skinny QR factorization $X = QR$ with the $B$-inner product using Householder reflections. Algorithmic variants as well as strategies for constructing an initial orthonormal basis are discussed. Theoretical analysis and numerical experiments demonstrate that Householder orthogonalization is numerically stable under mild assumptions over $B$, even if $X$ is rank deficient.

The rounding error analysis in this paper focuses on the numerical orthogonality. Rounding errors on the residual norm are only reported without theoretical analysis in this work. A more complete analysis regarding the Householder orthogonalization process, especially for difference between right-looking and left-looking variants, with and without the reorthogonalization step, will be helpful for better understanding the proposed methods. The robustness of Householder orthogonalization provides opportunities for new algorithmic variants for solving weighted least squares problems and generalized eigenvalue problems. Developments in these directions are planned as our future work.

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Appendix—Proof of Theorem 4

In order to prove Theorem 4 we first establish Lemma 5 for the rounding error of applying a Householder reflection to a vector in finite precision arithmetic. We assume that $(I_n - 2w\hat{w}^HB)y$ is computed through $\eta = \hat{w}^HB\hat{w}$ and then $y - 2\eta\hat{w}$.

**Lemma 5.** Let $B \in \mathbb{C}^{n \times n}$ be positive definite. Suppose that $z = (I_n - 2w\hat{w}^HB)y$ with $|\hat{w}^HB\hat{w} - 1| \leq \epsilon_n < 1$ and $w = \hat{w} / \|\hat{w}\|_B$. Under the assumption (15), there exists $\Delta H \in \mathbb{F}^{n \times n}$ such that $\text{fl}(z) = (I_n - 2w\hat{w}^HB + \Delta H)y$ and

$$
\|\Delta H\|_B = \|B^{1/2}\Delta HB^{-1/2}\|_2 \leq \delta,
$$

where

$$
\delta = 2\epsilon_n + (1 + 2\epsilon_n)\kappa_2(B)^{1/2}u
+ 2(1 + \kappa_2(B)^{1/2}u)(1 + \epsilon_n)(\kappa_2(B)\epsilon_B + (1 + \kappa_2(B)\epsilon_B)\kappa_2(B)^{1/2}u).
$$

**Proof.** For simplicity, within this proof we use $\varepsilon = \text{fl}(\cdot)$ interchangeably without further clarification. Let $\eta = \hat{w}^HBy$. We have $\hat{\eta} = \hat{w}^H(B + \Delta B)y$ with $\|\Delta B\|_2 \leq \epsilon_B \|B\|_2$. Then

$$
|\hat{\eta} - \eta| \leq \|B^{1/2}\hat{w}\|_2\|BB^{-1/2}\Delta BB^{-1/2}\|_2\|B^{1/2}y\|_2 \leq (1 + \epsilon_n)^{1/2}\kappa_2(B)\epsilon_B\|y\|_B,
$$

and

$$
|\hat{\eta}| \leq |\eta| + |\hat{\eta} - \eta| \leq \|\hat{w}\|_B\|y\|_B + |\hat{\eta} - \eta| \leq (1 + \epsilon_n)^{1/2}(1 + \kappa_2(B)\epsilon_B)\|y\|_B.
$$
Let \( v = 2 \hat{\omega} \eta, \hat{v} = \text{fl}(v) = \text{fl}(2 \hat{\omega} \hat{\eta}) \). Then
\[
\|v - \hat{v}\|_B \leq \|v - 2 \hat{\omega} \hat{\eta}\|_B + \|2 \hat{\omega} \hat{\eta} - \hat{v}\|_B
\leq 2 \|\hat{\omega}\|_B \|\eta - \hat{\eta}\| + \|B^{1/2}\|_2 \|2 \hat{\omega} \hat{\eta} - \hat{v}\|_2
\leq 2 \|\hat{\omega}\|_B \|\eta - \hat{\eta}\| + u \|B^{1/2}\|_2 \|2 \hat{\omega} \hat{\eta}\|_2
\leq 2 \|\hat{\omega}\|_B \|\eta - \hat{\eta}\| + 2 \|\hat{\eta}\| \kappa_2(B)^{1/2} u \|\hat{\omega}\|_B
\leq 2(1 + \epsilon_n) (\kappa_2(B) \epsilon_B + (1 + \kappa_2(B) \epsilon_B) \kappa_2(B)^{1/2} u) \|\hat{\omega}\|_B.
\]

Note that
\[
\|(I_n - 2 \hat{\omega} \hat{\omega}^H B) - (I_n - 2 w w^H B)\|_B = \|\hat{\omega}^H B \hat{\omega} - 1\| \cdot \|2 w w^H B\|_B \leq 2 \epsilon_n.
\]

We obtain
\[
\|z\|_B \leq \|(I_n - 2 w w^H B) y\|_B + \|(I_n - 2 \hat{\omega} \hat{\omega}^H B) y - (I_n - 2 w w^H B) y\|_B \leq (1 + 2 \epsilon_n) \|y\|_B.
\]

The forward error for evaluating \( z \) is given by
\[
r = z - z = \text{fl}(y - \hat{v}) - (y - \hat{v}) + (v - \hat{v}).
\]

Hence
\[
\|r\|_B \leq \|\text{fl}(y - \hat{v}) - (y - \hat{v})\|_B + \|v - \hat{v}\|_B
\leq \|B^{1/2}\|_2 \|\text{fl}(y - \hat{v}) - (y - \hat{v})\|_2 + \|v - \hat{v}\|_B
\leq u \|B^{1/2}\|_2 \|\hat{\omega} - \hat{v}\|_2 + \|v - \hat{v}\|_B
\leq \kappa_2(B)^{1/2} u \|\hat{\omega} - \hat{v}\|_B + \|v - \hat{v}\|_B
\leq (1 + 2 \epsilon_n) \kappa_2(B)^{1/2} u \|\hat{\omega}\|_B + (1 + \kappa_2(B)^{1/2} u) \|\hat{\omega}\|_B.
\]

Without loss of generality, we assume that \( y \neq 0 \). Let \( \Delta \hat{H} = y \hat{H} / (y^H B y) \). It is easy to verify that
\[
(I_n - 2 \hat{\omega} \hat{\omega}^H B + \Delta \hat{H}) y = z + r = \hat{z}
\]
and
\[
\|\Delta \hat{H}\|_B = \|r\|_B / \|y\|_B
\leq (1 + 2 \epsilon_n) \kappa_2(B)^{1/2} u + 2(1 + \kappa_2(B)^{1/2} u)(1 + \epsilon_n)(\kappa_2(B) \epsilon_B + (1 + \kappa_2(B) \epsilon_B) \kappa_2(B)^{1/2} u).
\]

By setting
\[
\Delta H = \Delta \hat{H} + (I_n - 2 \hat{\omega} \hat{\omega}^H B) - (I_n - 2 w w^H B),
\]
we arrive at the conclusion. \( \square \)

The following Lemma [6] provides the tool to analyze the error for evaluating a sequence of Householder reflections.

**Lemma 6.** Let \( H_i = I_n - 2 w_i w_i^H B \) with \( \|w_i\|_B = 1 \) for \( i = 1, 2, \ldots, k \). Then
\[
\|(H_1 + \Delta H_1)(H_2 + \Delta H_2) \cdots (H_k + \Delta H_k) y - H_1 H_2 \cdots H_k y\|_B \leq (1 + \delta)^k - 1 \|y\|_B,
\]
for \( \delta \geq \max_{1 \leq i \leq k} \|\Delta H_i\|_B \).

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Proof. Notice that $\tilde{H}_i = B^{1/2}H_iB^{-1/2}$ is a unitary matrix for $i = 1, 2, \ldots, k$. It follows from Lemma 3.7 that
\[
\|(H_1 + \Delta H_1) \cdots (H_k + \Delta H_k) - H_1 \cdots H_k\|_B \\
= \|(\tilde{H}_1 + B^{1/2}\Delta H_1B^{-1/2}) \cdots (\tilde{H}_k + B^{1/2}\Delta H_kB^{-1/2}) - \tilde{H}_1 \cdots \tilde{H}_k\|_2 \\
\leq \left(\prod_{i=1}^k (1 + \|B^{1/2}\Delta H_iB^{-1/2}\|_2) - 1\right) \prod_{i=1}^k \|\tilde{H}_i\|_2 \\
\leq (1 + \delta)^k - 1.
\]
Therefore,
\[
\|(H_1 + \Delta H_1)(H_2 + \Delta H_2) \cdots (H_k + \Delta H_k)y - H_1H_2 \cdots H_ky\|_B \\
\leq \|(H_1 + \Delta H_1)(H_2 + \Delta H_2) \cdots (H_k + \Delta H_k) - H_1H_2 \cdots H_k\|_B \|y\|_B \\
\leq ((1 + \delta)^k - 1) \|y\|_B.
\]

Now we are ready to proof Theorem 4. Let us define $\delta$ as in (18). It follows from Lemmas 5 and 6 that
\[
\|B^{1/2}\hat{q}_i - B^{1/2}(\tilde{H}\tilde{u}_i)\|_2 = \|\hat{q}_i - \tilde{H}\tilde{u}_i\|_B \leq ((1 + \delta)^k - 1) \|\tilde{u}_i\|_B \leq (1 + \epsilon)\frac{1}{2}((1 + \delta)^k - 1),
\]
where $\hat{q}_i$ and $\tilde{u}_i$ denote the $i$th columns of $\tilde{Q}$ and $\tilde{U}$, respectively. Therefore,
\[
\|B^{1/2}\hat{Q} - B^{1/2}(\tilde{H}\tilde{U})\|_2 \leq \|B^{1/2}\hat{Q} - B^{1/2}(\tilde{H}\tilde{U})\|_F \leq (1 + \epsilon)\frac{1}{2}((1 + \delta)^k - 1).
\]
It follows from Theorem 3 that
\[
\|B^{1/2}(\tilde{H}\tilde{U})\|_2 \leq \|(\tilde{H}\tilde{U})^H B(\tilde{H}\tilde{U})\|_2^{1/2} \leq (1 + \epsilon)\frac{1}{2}(1 + 4\kappa_2(1 + \epsilon)^{1/2}(1 + \delta)^k - 1).
\]

Using the inequality
\[
\|X^H X - Y^H Y\|_2 = \|(X - Y)^H Y + Y^H (X - Y)\|_2 \\
\leq 2\|(X - Y)^H Y\|_2 + \|(X - Y)^H (X - Y)\|_2 \\
\leq 2\|X - Y\|_2 \|Y\|_2 + \|X - Y\|_2^2,
\]
we obtain
\[
\|\hat{Q}^H B\hat{Q} - I_k\|_2 \leq \|\hat{Q}^H B\hat{Q} - (\tilde{H}\tilde{U})^H B(\tilde{H}\tilde{U})\|_2 + \|(\tilde{H}\tilde{U})^H B(\tilde{H}\tilde{U}) - I_k\|_2 \\
\leq 2\|B^{1/2}(\tilde{H}\tilde{U})\|_2 \|B^{1/2}(\hat{Q} - \tilde{H}\tilde{U})\|_2 + \|B^{1/2}(\hat{Q} - \tilde{H}\tilde{U})\|_2^2 \\
+ \|(\tilde{H}\tilde{U})^H B(\tilde{H}\tilde{U}) - I_k\|_2.
\]

Every term in the upper bound has already been analyzed.

In order to derive a neat estimate without high order terms such as $O((\epsilon_1^2)$, we make use of the inequality
\[
(1 + a)^b \leq \frac{1}{1 - ab}, \quad \text{if } a > 0, b > 0, ab < 1.
\]

Under the assumptions that $\epsilon_1 \leq 1$ and $18k\kappa_2(B)\epsilon_1 < 1$, we have
\[
\delta \leq \frac{568}{155}k\kappa_2(B)^{1/2} u + \frac{38}{17}k\kappa_2(B)\epsilon_1 + 2\epsilon_1 \leq 9\kappa_2(B)\epsilon_1,
\]
\[
(1 + \delta)^k - 1 \leq \frac{k\delta}{1 - k\delta} \leq 2k\delta \leq 18k\kappa_2(B)\epsilon_1 < 1,
\]

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and
\[(1 + \epsilon_n)^{4k-2} \leq \frac{1}{1 - 4k\epsilon_n} \leq \frac{17}{13}\]

Finally, we obtain
\[
\|\hat{Q}^\dagger B\hat{Q} - I_k\|_2 \leq 2(1 + \epsilon_o)^{1/2}(1 + 4k\epsilon_n(1 + \epsilon_n)^{4k-2})^{1/2} \cdot k^{1/2}(1 + \epsilon_o)^{1/2}(1 + \delta)^k - 1)
+ k(1 + \epsilon_n)((1 + \delta)^k - 1)^2 + \epsilon_o + 4k\epsilon_n(1 + \epsilon_o)(1 + \epsilon_n)^{4k-2}
\leq \epsilon_o + \frac{136}{13} k\epsilon_n + \frac{216}{\sqrt{13}} k^{3/2} \kappa_2(B)\epsilon_B + \frac{324}{17} k^2 \kappa_2(B)\epsilon_B
\]
\[
= \epsilon_o + O(k^2 \kappa_2(B)\epsilon_B).
\]

This completes the proof of Theorem 4.

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