Orthonormal Completion of an array of Unit Length Vectors

An effective approach to rounding error analyses of “iterative” orthogonalization algorithms

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Outline

1. What led to this work?
2. A unitary matrix
3. Relationship with Householder matrices
4. The Evolution of This Idea
5. The Barlow, Bosner and Drmač Bidiagonalization

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Their paper combined the two bidiagonalization algorithms in:

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Notation

SUT means "strictly upper triangular", (SLT –"lower").

$\mathrm{sut}(V_k^H V_k)$ is the SUT part of $V_k^H V_k$.

$\|x\| \equiv \sqrt{x^H x}$.

$\|A\|_2 = \sigma_{\max}(A)$, $\kappa_2(A) \equiv \sigma_{\max}(A)/\sigma_{\min}(A)$.

$\|A\|_F \equiv \sqrt{\mathrm{trace}(A^H A)}$.

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The Main Characters

Many numerical algorithms are designed to compute
a sequence of orthonormal vectors:

$$v_1, v_2, \ldots \in \mathbb{C}^n, \qquad V_k \equiv [v_1, \ldots, v_k] \in \mathbb{C}^{n\times k}, \quad V_k^H V_k = I_k.$$

But in Gram-Schmidt and related computations, usually

$$\|V_k^H V_k - I_k\|_F \quad \text{is not at all small.}$$

From now on let $v_1, v_2, \ldots \in \mathbb{C}^n$ be any sequence with:

$$\|v_j\| = 1, \quad j = 1, 2, \ldots; \qquad V_k \equiv [v_1, \ldots, v_k] \in \mathbb{C}^{n\times k}.$$

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The Main Result—Theory

The Simple Theorem

Theorem

For any $V \equiv [v_1, \dots, v_k] \in \mathbb{C}^{n\times k}$ *with* $\|v_j\| = 1, \;\; j = 1, \dots, k,$ *there exists a unique strictly upper triangular matrix*

$$S \equiv (I+U)^{-1}U \quad \in \mathbb{C}^{k\times k}, \qquad \textit{where} \quad U \equiv \mathrm{sut}(V^H V),$$

such that Q *is unitary in:*

$$Q \equiv [Q_1 \mid Q_2] \equiv \left[\begin{array}{c|c} S & (I-S)V^H \\ \hline V(I-S) & I - V(I-S)V^H \end{array}\right];$$

also $\quad 0 \le \|S\|_2 \le 1, \quad$ *and* $\left\{\begin{array}{l} V^H V = I \;\Leftrightarrow\; \|S\|_2 = 0, \\ V^H V \;\; \textit{singular} \;\Leftrightarrow\; \|S\|_2 = 1. \end{array}\right.$

$\|S\|_2$ is a superb measure of loss of orthogonality in $v_1, v_2, \dots, v_k$.

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Key Part of Proof

Given $V \in \mathbb{C}^{n\times k}$ with diag_of$(V^H V) = I$, let $S \in \mathbb{C}^{k\times k}$ be SUT.

Define $U \equiv \mathrm{sut}(V^H V)$, $Q_1 \equiv \begin{bmatrix} S \\ V(I-S) \end{bmatrix}$.

Then $Q_1^H Q_1 = I \quad \Leftrightarrow \quad \underline{S = (I+U)^{-1}U}$.

Proof: Since $V^H V = I + U + U^H$, for $M \equiv Q_1^H Q_1 - I$ we have

$$
\begin{aligned}
M &= S^H S + (I-S)^H(I-S) + \underline{(I-S)^H(U+U^H)(I-S)} - I \\
&= \underline{(I-S)^H(U+U^H)(I-S)} + S^H S + I - S - S^H(I-S) - I \\
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$$(I-S)^{-H} M (I-S)^{-1} = (U+U^H) - S(I-S)^{-1} - (I-S)^{-H} S^H.$$

But $U - S(I-S)^{-1}$ is SUT, so $M = 0$ if and only if

$U = S(I-S)^{-1}$ i.e. $S = U(I-S) = U - US$ so $\underline{(I+U)S = U}$.

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What does it matter?

One Use of this Result—Theory

Giraud & Langou, IMAJNA (2002), proved under mild conditions that V_k from MGS is well-conditioned.

The new theorem leads to the general result:
If $\|v_j\| = 1, \quad j = 1, \ldots, k, \quad V_k \equiv [v_1, \ldots, v_k]$, then

$$\sigma_{\min}(V_k) \geq \sqrt{\frac{1 - \|S_k\|_2}{1 + \|S_k\|_2}}, \quad \text{and} \quad \kappa_2(V_k) \leq \frac{1 + \|S_k\|_2}{1 - \|S_k\|_2}.$$

Bounding $\|S_k\|_2 < 1$ bounds $\kappa_2(V_k)$ for any orthogonalization algorithm! (Effectively what Giraud & Langou did for MGS).

V_k is well conditioned even when significant orthogonality is lost.
E.g. if $\|S_k\|_2 = .9$, (a severe loss of orthogonality in V_k), $\kappa_2(V_k) \leq 19$, which is surprisingly and pleasingly small.

Also we see how $\kappa_2(V_k) \to \infty$ as $\|S_k\|_2 \nearrow 1$.
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E.g. if $\|S_k\|_2 = .9$, (a severe loss of orthogonality in V_k), $\kappa_2(V_k) \leq 19$, which is surprisingly and pleasingly small.

Also we see how $\kappa_2(V_k) \to \infty$ as $\|S_k\|_2 \nearrow 1$.
$\|S_k\|_2$ is a superb measure of loss of orthogonality!

General Use of this Result—Practice

An algorithm produces $v_1^c, \ldots, v_k^c$, supposedly orthogonal, & almost normalized (since last computation for each v_j^c).

Let $\widetilde{V} \equiv [\tilde{v}_1, \ldots, \tilde{v}_k]$, where $\tilde{v}_j$ are the normalized v_j^c.

If we can find the ideal expression involving

$$S \equiv (I + U)^{-1} U \qquad \text{where} \quad U \equiv \mathrm{sut}(\widetilde{V}^H \widetilde{V}),$$

we might be able to show that the algorithm is backward stable for an augmented problem involving unitary

$$Q \equiv \left[\begin{array}{c|c} S & (I-S)\widetilde{V}^H \\ \hline \widetilde{V}(I-S) & I-\widetilde{V}(I-S)\widetilde{V}^H \end{array}\right].$$

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The Simple Theorem, with indexing

Theorem

For any $V_k \equiv [v_1, \ldots, v_k] \in \mathbb{C}^{n\times k}$ *with* $\|v_j\| = 1, \;\; j = 1, \ldots, k$, *there exists a unique strictly upper triangular matrix*

$$S_k \equiv (I_k + U_k)^{-1} U_k, \qquad \textit{where} \quad U_k \equiv \mathrm{sut}(V_k^H V_k),$$

such that $Q^{(k)}$ *is unitary, where:*

$$Q^{(k)} \equiv \left[Q_1^{(k)} \;\middle|\; Q_2^{(k)} \right] \equiv \left[\begin{array}{c|c} S_k & (I_k - S_k) V_k^H \\ \hline V_k (I_k - S_k) & I_n - V_k (I_k - S_k) V_k^H \end{array} \right].$$

The change in $Q^{(k)}$ when append v_{k+1}.

With $s_{k+1} \equiv (I_k - S_k)u_{k+1}$, $u_{k+1} \equiv V_k^H v_{k+1}$, we have

$$V_{k+1} = [V_k, v_{k+1}], \qquad S_{k+1} = \left[\begin{array}{c|c} S_k & s_{k+1} \\ \hline 0 & 0 \end{array}\right],$$

$$Q_1^{(k+1)} \equiv \left[\begin{array}{c} S_{k+1} \\ \hline V_{k+1}(I_{k+1} - S_{k+1}) \end{array}\right] = \left[\begin{array}{c|c} S_k & s_{k+1} \\ 0 & 0 \\ \hline V_k(I_k - S_k) & v_{k+1} - V_k s_{k+1} \end{array}\right].$$

We see that

$$Q^{(k)} \equiv \left[Q_1^{(k)} \;\middle|\; Q_2^{(k)}\right] \equiv \left[\begin{array}{c|c} S_k & (I_k - S_k)V_k^H \\ \hline V_k(I_k - S_k) & I_n - V_k(I_k - S_k)V_k^H \end{array}\right]$$

is $(n+k) \times (n+k)$, so our sequence $v_1, \ldots, v_k$
can go on forever, and we *always* have unitary matrices $Q^{(k)}$.

Think of the Lanczos process,
and Hestenes' & Steifel's method of conjugate gradients.

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The Householder connection

Relationship with Householder matrices

Theorem

For any $V \equiv [v_1, \ldots, v_k] \in \mathbb{C}^{n\times k}$ *with* $\|v_j\| = 1, \;\; j = 1, \ldots, k,$

define $p_j \equiv \begin{bmatrix} -e_j \\ v_j \end{bmatrix} \in \mathbb{C}^{n+k}, \qquad P^{(j)} \equiv I_{n+k} - p_j p_j^H,$

then the $P^{(j)}$ *are Householder matrices, and with*

$$S \equiv (I+U)^{-1}U \qquad \textit{where} \qquad U \equiv \mathrm{sut}(V^H V),$$

we have:

$$Q \;\equiv\; \left[\begin{array}{c|c} S & (I-S)V^H \\ \hline V(I-S) & I-V(I-S)V^H \end{array}\right] \;=\; P^{(1)}P^{(2)}\ldots P^{(k)}.$$

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The Evolution of This Idea

Charles Sheffield

Charles Sheffield realized the modified Gram–Schmidt (MGS) orthogonalization algorithm for the QR factorization of $B \in \mathbb{R}^{n \times k}$ is numerically equivalent to the Householder QR factorization applied to the $(n+k) \times k$ matrix $\begin{bmatrix} 0 \\ B \end{bmatrix}$.

Sheffield's observation was applied by:

Björck & Paige (1992, 1994) in their stability analyses of MGS;

Giraud & Langou (2002) to prove V_k well-conditioned in MGS;

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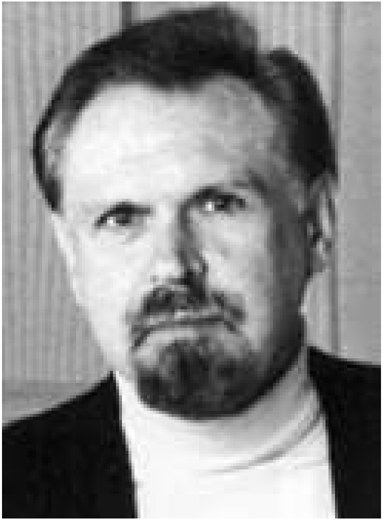
Charles Sheffield, June 1935 – November 2002



Sheffield's Observation, continued.

It was originally assumed that the idea, and the structure of $P^{(1)} \dots P^{(k)} = Q^{(k)}$, was only relevant to the MGS algorithm.

We now see it is useful for analyzing any algorithm which in theory produces orthonormal vectors, but in practice, because of rounding errors, can fail to do so to a significant extent.

Since the ideas can be applied to any sequence of unit length n-vectors, MGS is just a particular, but remarkable, case.

The theorem offers hope for the successful rounding error analyses of other important algorithms, such as:
the eigenvalue algorithm of Lanczos,
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Bidiagonalization Algorithms

Bidiagonalization—one important use

Now we switch to REALS

Orthogonally transform the given matrix X
so that with orthogonal matrices V and W:

$V^TXW \quad \rightarrow \quad$ bidiagonal B, a direct computation,
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Golub & Kahan

Direct & "Iterative"

Bidiagonalization

Direct upper bidiagonalization (ubd) of $n \times m$ X, $n \geq m$:

$$V^T X\ W = \begin{bmatrix} B \\ 0 \end{bmatrix}; \quad B \equiv \begin{bmatrix} \beta_1 & \alpha_1 & & \\ & \beta_2 & \cdot & \\ & & \cdot & \alpha_{m-1} \\ & & & \beta_m \end{bmatrix}, \quad m \times m.$$

$$V^T X\ W \quad = \quad V^{(m)} \ldots V^{(3)} V^{(2)} V^{(1)} \quad X \quad W^{(1)} W^{(2)} \ldots W^{(m)}$$

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Combined
Direct & "Iterative"
Bidiagonalization

BBD: Barlow, Bosner & Drmač, (LAA 2005),
"A new stable bidiagonal reduction algorithm"

Direct & "Iterative" bidiagonalizations.

1. Golub & Kahan Direct algorithm $V^T X W = \left[\begin{smallmatrix} B \\ 0 \end{smallmatrix}\right]$, $n \times m$:
stops in m steps and is backward stable;
ideal for small to moderately large dimensioned X.

2. Golub & Kahan Iterative algorithm: v_j, w_j "iterative"
$\longrightarrow$ loses orthogonality $\longrightarrow$ NO m-step termination;
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3. BBD Direct & "Iterative" alg.: $W^{(j)}$ Householder matrices
$\longrightarrow$ m-step termination; v_j "iteratively", lose orthogonality.
Can be faster than Direct algorithm.
Useful for moderately large problems where do not need orthogonality in all "left" singular vectors of X
(from rounding error analysis of the algorithm).

All 3 algorithms $\longrightarrow$ accurate singular values to $O(\epsilon)\|X\|_2$.

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A Rounding Error Result

REA of BBD Bidiagonalization $V_m^T X W = B$

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Ideally: $V_m^T V_m = I_m$, $W^{-1} = W^T$, bidiagonal B.

Computationally: have $\widetilde{V}_m$ (correctly normalized), $\widetilde{B}$, $\widetilde{W}$.

One REA result: Let $U \equiv \mathrm{sut}(\widetilde{V}_m^T \widetilde{V}_m)$.

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