What do we know about block Gram-Schmidt?

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The Gram-Schmidt process

Given a set of linear independent vectors $x_1, \ldots, x_n$, we want to compute a set of orthogonal vectors $q_1, \ldots q_n$ such that $span\{x_1, \ldots, x_n\} = span\{q_1, \ldots, q_n\}$
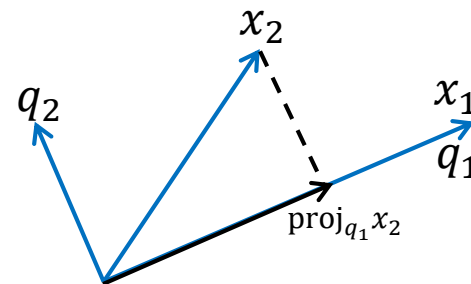
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Gram-Schmidt process:

$$q_1 = x_1, \ \ q_k = x_k - \sum_{j=1}^{k-1} \frac{\langle q_j, x_k \rangle}{\|q_j\|^2} q_j, \ \ k \geq 2$$

To get orthonormal vectors, $q_k = q_k / \|q_k\|$, for all k

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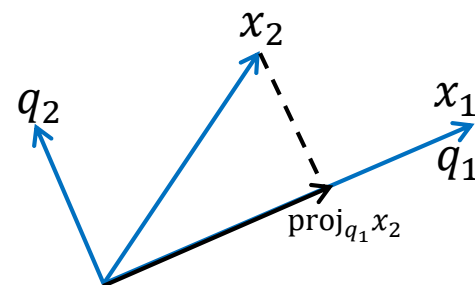To get orthonormal vectors, $q_k = q_k / \|q_k\|$, for all k

Each vector x_k can be expressed as a linear combination of $q_1, \ldots, q_k$.

So with $X = [x_1 \cdots x_n]$, $Q = [q_1 \cdots q_n]$, this means we can write
$$X = QR,$$

Where columns of R give the coefficients of the aforementioned linear combinations, and thus R is upper triangular.

Typically require that the diagonal entries of R are positive; this gives a unique QR factorization.

Orthogonalization

- Many applications
  - Solving least squares problems $\min_{x} \|Ax - b\|_2^2 \quad \rightarrow \quad Rx = Q^T b$
  - Used within Krylov subspace methods
  - Etc.

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  - Householder, Givens rotations, Tall-Skinny QR (TSQR), CholeskyQR, …

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- What happens in finite precision?
  - On a real computer, every time we perform a floating point operation, we may incur a small roundoff error
  - Over a whole computation, these tiny errors can accumulate or can be amplified!
  - The result:
    - $\bar{Q}$ no longer has exactly orthonormal columns!
    - $\bar{Q}\bar{R}$ is no longer exactly the same as X!
      - This can affect applications downstream

Measures of Error

Let $\bar{Q}$ and $\bar{R}$ denote computed QR factors of a matrix X.

How far is $\bar{Q}$ from being orthogonal?

"Loss of orthogonality": $\|I - \bar{Q}^T\bar{Q}\|$

How close is $\bar{Q}\bar{R}$ to X?

Relative residual norm: $\dfrac{\|X - \bar{Q}\bar{R}\|}{\|X\|}$

How close is $\bar{R}^T\bar{R}$ to X^TX?

Relative Cholesky residual norm: $\dfrac{\|X^TX - \bar{R}^T\bar{R}\|}{\|X\|^2}$

Gram-Schmidt algorithms

Classical Gram-Schmidt (CGS)

for $k = 1, \ldots, n$
    $w_k = x_k$
    for $j = 1, \ldots, k-1$
        $w_k = w_k - (q_j^T x_k) q_j$
    $q_k = w_k / \|w_k\|$

Modified Gram-Schmidt (MGS)

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	CGS	MGS
Computation of entries of R	$r_{jk} = q_j^T x_k$	$r_{jk} = q_j^T \left(x_k - \sum_{i=1}^{k-1} r_{ik} q_k \right)$
Computation of next orthogonal vector	$\left(I - Q_{1:k-1} Q_{1:k-1}^T\right) x_k$	$\left(I - q_{k-1} q_{k-1}^T\right) \cdots \left(I - q_1 q_1^T\right) x_k$
Parallel messages/ synchronizations	$O(1)$	$O(k)$ in loop k
Loss of orthogonality	$\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon) \kappa^{n-1}(X)$ if $O(\varepsilon)\kappa(X) < 1$	$\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon) \kappa(X)$ if $O(\varepsilon)\kappa(X) < 1$

A bit of history…

[Leon, Björck, Gander, "Gram-Schmidt orthogonalization: 100 years and more", 2007]

- Method of orthogonalization popularized by a paper of Schmidt in 1907. The method here is what we know as "classical Gram-Schmidt"

- In a footnote, Schmidt credits an earlier paper by Gram, published in 1883, saying that this procedure is essentially equivalent.
  - The procedure in Gram's paper is what we know as "modified Gram-Schmidt"

- The linkage of the names "Gram" and "Schmidt" came along in 1935 in a paper by Wong

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Jørgen Pedersen Gram   Erhard Schmidt   Pierre-Simon Laplace

- It turns out a procedure equivalent to modified Gram-Schmidt appears even in much earlier work of Laplace in 1820

Block Gram-Schmidt

- Sometimes we may want to use a block version of Gram-Schmidt

- Performance reasons (e.g., BLAS3)
- Block Krylov subspace methods
    - Better convergence
    - Simultaneously solve multiple RHSes
- s-step Krylov subspace methods

Muscle and Skeleton analogy   [Hoemmen, 2010]
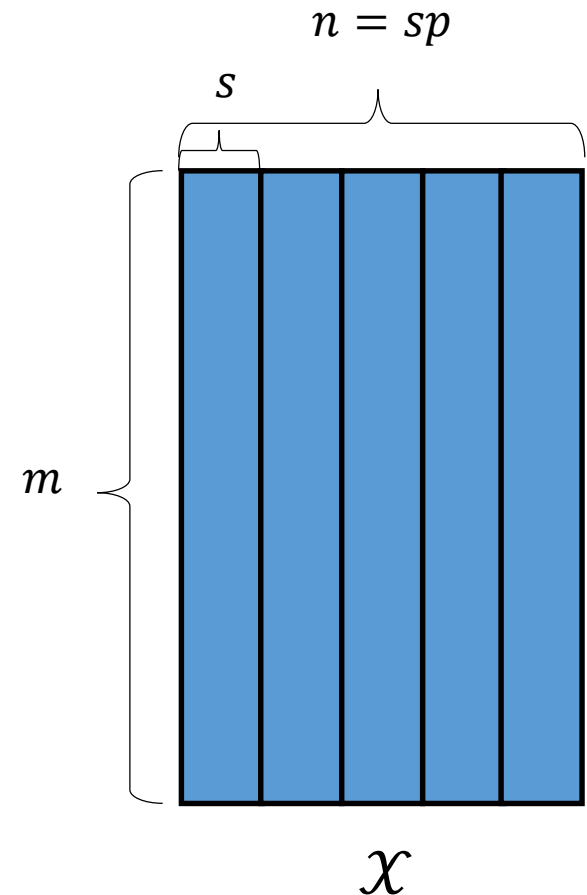
- How do we define a block Gram-Schmidt algorithm?

- We need 2 parts:
  - The "skeleton": A block Gram-Schmidt algorithm for interblock orthogonalization
  - The "muscle": A non-block orthogonalization algorithm for intrablock orthogonalization ("local QR", "panel factorization")
    - Need not be Gram-Schmidt-based
    - We will refer to this routine as "IntraOrtho()"

https://www.twinkl.com/illustration/contracted-muscle-arm-bone-skeleton-movement-anatomy-bicep-science-ks2

- For example: block MGS (BMGS) for orthogonalizing between blocks, Householder QR for orthogonalizing within blocks:

$$\text{BMGS} \circ \text{HouseQR}(\mathcal{X})$$
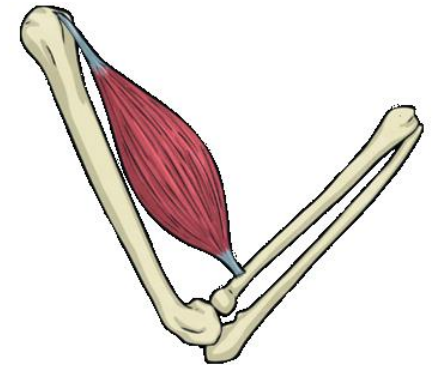
Notation I

- Use our own naming system of algorithms
  - Does suffix "2" mean reorthogonalized? BLAS-2 featuring? A second version of the algorithm?

- Suffixes:
  - +: run twice
  - I+: inner reorthogonalization
  - S+: selective reorthogonalization

Notation II

- Calligraphic letters for the whole block matrices $(\mathcal{X}, \mathcal{Q}, \mathcal{R})$
- Regular letters for the individual block quantities (X, Q, R)
- Bars denote computed (inexact) quantities

- m: number of rows in input matrix
- n: number of columns in input matrix $(n = ps)$
- p: number of blocks
- s: number of columns per block

$$m \geq n > p > s$$

$$\mathcal{X} = [X_1, X_2, \ldots, X_p], \quad \mathcal{X} \in \mathbb{R}^{m \times n}, \quad X_i \in \mathbb{R}^{m \times s}$$

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Economic QR factorization: $\mathcal{X} = \mathcal{Q}\mathcal{R}$, $\mathcal{Q} \in \mathbb{R}^{m \times n}, \mathcal{R} \in \mathbb{R}^{n \times n}$

$$\mathcal{Q} = [Q_1, Q_2, \ldots, Q_p], \quad \mathcal{R} = \begin{bmatrix} R_{1,1} & R_{1,2} & \cdots & R_{1,p} \\ & R_{2,2} & \cdots & R_{2,p} \\ & & \ddots & \vdots \\ & & & R_{p,p} \end{bmatrix}$$

$$\mathcal{Q}_{1:j} = [Q_1, \ldots, Q_j], \quad \mathcal{R}_{1:j,k} = \begin{bmatrix} R_{1,k} \\ \vdots \\ R_{j,k} \end{bmatrix}$$

Block Gram-Schmidt methods in practice

A few examples:

- [Boley and Golub, 1984]: Block Arnoldi with BMGSI+ ∘ MGSI+

  "However, since we obtain Z_k, by using a [block] Gram-Schmidt orthogonalization of W_k, against $Q_1, ..., Q_k$ ... there is little loss of stability by continuing to use Gram-Schmidt to orthogonalize Z_k. This was what we actually observed in our numerical experiments."

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- [Sadkane, 1993]: Block Arnoldi with BMGS ∘ "QR factorization"

- [Saad, 2003]: textbook provides block Arnoldi based on BCGS (Alg. 6.22) and BMGS (Alg. 6.23); IntraOrtho just specified as a "QR factorization"

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- Does it matter what we use for "QR factorization" (the IntraOrtho) within a block Gram-Schmidt method?

Does it matter?

- Recall: For MGS, $\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)\kappa(X)$

- What is the bound on loss of orthogonality for BMGS ∘ MGS? (guess!)

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Läuchli matrix

$$\boldsymbol{\mathcal{X}} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ \eta & & & \\ & \eta & & \\ & & \ddots & \\ & & & \eta \end{bmatrix}$$

$$\eta \in (\varepsilon, \sqrt{\varepsilon})$$

$$m = 1000, p = 100, s = 5$$

[Jalby and Philippe, 1991]: For BMGS ∘ MGS, $\|I - \bar{Q}^T\bar{Q}\| \leq O(\varepsilon)\kappa^2(\mathcal{X})$

`LaeuchliBlockKappaPlot([1000 100 5], logspace(-1, -16, 10), {'BMGS'}, {'MGS'})`

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LaeuchliBlockKappaPlot([1000 100 5], logspace(-1, -16, 10), {'BMGS'}, {'MGS', 'MGS_IRO'})

If we use an intrablock orthogonalization routine (muscle) with $O(\varepsilon)$ loss of orthogonality and $O(\varepsilon)$ relative residual, what is the best a block Gram-Schmidt orthogonalization routine (skeleton) can do?

For a given block Gram-Schmidt variant (skeleton), what are the minimum requirements on the intra-block orthogonalization routine (muscle) such that the loss of orthogonality is good enough?

BlockStab MATLAB package

BlockStab (our code) has two simple drivers:

- BGS(XX, s, skel, musc, rpltol, verbose)
- IntraOrtho(X, musc, rpltol, verbose)
- Can also work directly with a skeleton or muscle, or implement your own

https://github.com/katlund/BlockStab

For each plot, we list the function call needed to replicate the plot at the bottom of the slide

Outline

1. Overview of muscles
2. BCGS skeletons
3. BMGS skeletons
4. Open questions

Overview of Muscles

CGS and CGS-P

- Pessimistic bound due to [Kiełbasiński, 1974]: If $O(\varepsilon)\kappa(X) < 1$,

$$\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)\kappa^{s-1}(X)$$

for $X \in \mathbb{R}^{m \times s}$

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- [Giraud, Langou, Rozložník, van den Eshof, 2005]: If $O(\varepsilon)\kappa^2(X) < 1$,

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$$R_{1:k,k+1} = Q_{1:k}^T x_{k+1}$$
$$w = x_{k+1} - Q_{1:k}R_{1:k,k+1}$$

Let $\phi = \|x_{k+1}\|, \;\; \psi = \|R_{1:k,k+1}\|$

CGS:
$$R_{k+1,k+1} = \|w\| \left(= \sqrt{\phi^2 - \psi^2}\right)$$

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CGS-P:
$$R_{k+1,k+1} = \sqrt{\phi - \psi} \cdot \sqrt{\phi + \psi}$$

Reorthogonalization

- "Twice is enough"

  [Parlett, 1987]; attributed to Kahan :

  An iterative Gram-Schmidt process on 2 vectors with one step of reorthogonalization produces 2 vectors orthonormal up to machine precision *if the matrix is not too ill-conditioned.*

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- [Giraud, Langou, Rozložník, 2002], [Giraud, Langou, Rozložník, van den Eshof, 2005]: Twice is enough holds for $k > 2$ vectors
  - Previous work by [Abdelmalek, 1971]

$$\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)$$

- Many variants: CGS+, CGSI+, CGSS+

Low-synchronization version

CGSI+LS [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2020]

- One synchronization per column (CGSI+ up to 4)

$[\boldsymbol{Q}, R] = \texttt{CGSI+LS}(\boldsymbol{X})$

1: Allocate memory for $\boldsymbol{Q}$ and R
2: $\boldsymbol{u} = \boldsymbol{x}_1$
3: **for** $k = 2, \ldots s$ **do**
4:     **if** $k = 2$ **then**
5:         $[r_{k-1,k-1}^2 \ \rho] = \boldsymbol{u}^T[\boldsymbol{u} \ \boldsymbol{x}_k]$
6:     **else if** $k > 2$ **then**
7:         $\begin{bmatrix} \boldsymbol{w} & \boldsymbol{z} \\ \omega & \zeta \end{bmatrix} = [\boldsymbol{Q}_{1:k-2} \ \boldsymbol{u}]^T[\boldsymbol{u} \ \boldsymbol{x}_k]$
8:         $[r_{k-1,k-1}^2 \ \rho] = [\omega \ \zeta] - \boldsymbol{w}^T[\boldsymbol{w} \ \boldsymbol{z}]$
9:     **end if**
10:    $r_{k-1,k} = \rho/r_{k-1,k-1}$
11:    **if** $k = 2$ **then**
12:        $\boldsymbol{q}_{k-1} = \boldsymbol{u}/r_{k-1,k-1}$
13:    **else if** $k > 2$ **then**
14:        $R_{1:k-2,k-1} = R_{1:k-2,k-1} + \boldsymbol{w}$
15:        $R_{1:k-2,k} = \boldsymbol{z}$
16:        $\boldsymbol{q}_{k-1} = (\boldsymbol{u} - \boldsymbol{Q}_{1:k-2}\boldsymbol{w})/r_{k-1,k-1}$
17:    **end if**
18:    $\boldsymbol{u} = \boldsymbol{x}_k - \boldsymbol{Q}_{1:k-1}R_{1:k-1,k}$
19: **end for**
20: $\begin{bmatrix} \boldsymbol{w} \\ \omega \end{bmatrix} = [\boldsymbol{Q}_{1:s-1} \ \boldsymbol{u}]^T\boldsymbol{u}$
21: $r_{s,s}^2 = \omega - \boldsymbol{w}^T\boldsymbol{w}$
22: $R_{1:s-1,s} = R_{1:s-1,s} + \boldsymbol{w}$
23: $\boldsymbol{q}_s = (\boldsymbol{u} - \boldsymbol{Q}_{1:s-1}\boldsymbol{w})/r_{s,s}$
24: **return** $\boldsymbol{Q} = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_s]$, $R = (r_{jk})$

Low-synchronization version

CGSI+LS [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2020]

- One synchronization per column (CGSI+ up to 4)

Main ideas:

1. Compute strictly lower triangular matrix L one row (or block of rows) at a time in single reduction to compute all inner products needed for current iteration

$$L_{k-1,1:k-2} = \left(Q_{1:k-2}^T q_{k-1}\right)^T$$

2. "Lag" normalization step and merge it with this single reduction
   - Idea of delay also used in [Hernández, Román, Tomás, 2007]

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8:     $[r_{k-1,k-1}^2 \ \rho] = [\omega \ \zeta] - \boldsymbol{w}^T [\boldsymbol{w} \ \boldsymbol{z}]$
9:   end if
10:   $r_{k-1,k} = \rho / r_{k-1,k-1}$
11:   if $k = 2$ then
12:     $\boldsymbol{q}_{k-1} = \boldsymbol{u} / r_{k-1,k-1}$
13:   else if $k > 2$ then
14:     $R_{1:k-2,k-1} = R_{1:k-2,k-1} + \boldsymbol{w}$
15:     $R_{1:k-2,k} = \boldsymbol{z}$
16:     $\boldsymbol{q}_{k-1} = (\boldsymbol{u} - \boldsymbol{Q}_{1:k-2}\boldsymbol{w}) / r_{k-1,k-1}$
17:   end if
18:   $\boldsymbol{u} = \boldsymbol{x}_k - \boldsymbol{Q}_{1:k-1} R_{1:k-1,k}$
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22: $R_{1:s-1,s} = R_{1:s-1,s} + \boldsymbol{w}$
23: $\boldsymbol{q}_s = (\boldsymbol{u} - \boldsymbol{Q}_{1:s-1}\boldsymbol{w}) / r_{s,s}$
24: return $\boldsymbol{Q} = [\boldsymbol{q}_1, \ldots, \boldsymbol{q}_s]$, $R = (r_{jk})$

Low-synchronization version: details

Observation of Ruhe [1983]: MGS = Gauss-Seidel iteration, CGS = Gauss-Jacobi iterations for solving the normal equations.

Associated orthogonal projector:

$$I - Q_{1:k-1}T_{1:k-1,1:k-1}Q_{1:k-1}^T \quad \text{for} \quad T_{1:k-1,1:k-1} \approx \left(Q_{1:k-1}^T Q_{1:k-1}\right)^{-1}$$

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For CGSI+LS (see [Świrydowicz, et al., 2020] for details)

$$T_{1:k-1,1:k-1} = I - L_{1:k-1,1:k-1} - L_{1:k-1,1:k-1}^T$$

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$$T_{1:k-1,1:k-1} = I - L_{1:k-1,1:k-1} - L_{1:k-1,1:k-1}^T$$

In each CGSI+LS step, split $T_{1:k-1,1:k-1}$ into two parts, apply them across two iterations

- Apply $I - L_{1:k-1,1:k-1}$
- Apply (lagged) correction: $R_{1:k-2,k-1} = R_{1:k-2,k-1} - L_{1:k-1,1:k-2}^T$

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⇒Reorthogonalization happens "on the fly" instead of requiring complete second pass

Summary: CGS Variants

Algorithm	$\|I - \bar{Q}^T \bar{Q}\|$	Assumption on $\kappa(X)$	References
CGS	$O(\varepsilon)\kappa^{n-1}(X)$	$O(\varepsilon)\kappa(X) < 1$	[Kiełbasiński, 1974]
CGS-P	$O(\varepsilon)\kappa^2(X)$	$O(\varepsilon)\kappa^2(X) < 1$	[Smoktunowicz, Barlow, Langou, 2006]
CGS+	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	conjecture
CGSI+	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	[Abdelmalek, 1971] [Giraud, Langou, Rozložník, 2002] [Giraud, Langou, Rozložník, van den Eshof, 2005] [Barlow, Smoktunowicz, 2013]
CGSS+	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	[Daniel, Gragg, Kaufman, Stewart, 1976] [Hoffmann, 1989]
CGSI+LS	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	conjecture [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2020]
CGSS+rpl	$O(\varepsilon)$	none	conjecture [Stewart, 2008]

Low-sync MGS

- Original low-sync muscles developed independently by [Świrydowicz et al., 2020] and [Barlow 2019]

- Perspectives:
  - Merge inner products and norms by batching and lagging
  - Cushion MGS projectors with "error sponge" to achieve CGS-like communication with MGS-like stability

$$\text{CGS:} \quad \left(I - Q_k Q_k^T\right) x_{k+1}$$

$$\text{MGS:} \quad \left(I - q_k q_k^T\right) \cdots \left(I - q_1 q_1^T\right) x_{k+1}$$

$$\text{Goal:} \quad \left(I - Q_k \textcolor{red}{C_k} Q_k^T\right) x_{k+1}$$

Low-sync variants

	Two synchronizations	One synchronization
$\left(I - Q_k T_k^T Q_k^T\right) x_{k+1}$ (matrix-matrix multiplication)	MGS-SVL [Barlow, 2019] (called "MGS2")	MGS-CWY [Swirydowicz et al., 2020]
$\left(I - Q_k T_k^{-T} Q_k^T\right) x_{k+1}$ (triangular solve)	MGS-LTS [Swirydowicz et al., 2020]	MGS-ICWY [Swirydowicz et al., 2020]

Low-sync variants

[Schreiber and Van Loan, 1989]   + "Sheffield observation"

	Two synchronizations	One synchronization
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[Puglisi, 1992]
[Björck, 1994]

Low-sync variants

[Schreiber and Van Loan, 1989]   + "Sheffield observation"

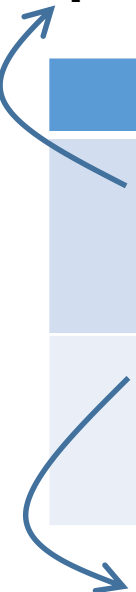|	Two synchronizations	One synchronization
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[Puglisi, 1992]
[Björck, 1994]

Note: For block variants, it will be a crucial point that these algorithms return T_k

MGS Variants

Algorithm	$\|I - \bar{Q}^T \bar{Q}\|$	Assumption on $\kappa(X)$	References
MGS	$O(\varepsilon)\kappa(X)$	$O(\varepsilon)\kappa(X) < 1$	[Björck, 1967]
MGS-SVL	$O(\varepsilon)\kappa(X)$	$O(\varepsilon)\kappa(X) < 1$	[Barlow, 2019]
MGS-LTS	$O(\varepsilon)\kappa(X)$	$O(\varepsilon)\kappa(X) < 1$	conjecture [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2020]
MGS-CWY	$O(\varepsilon)\kappa(X)$	$O(\varepsilon)\kappa(X) < 1$	conjecture [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2020]
MGS-ICWY	$O(\varepsilon)\kappa(X)$	$O(\varepsilon)\kappa(X) < 1$	conjecture [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2020]
MGS+	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	[Jalby, Philippe, 1991] [Giraud, Langou, 2002]
MGSI+	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	[Hoffmann, 1989] [Gander, 1980] [Giraud, Langou, Rozložník, 2002]

Other Muscles

Algorithm	$\|I - \bar{Q}^T \bar{Q}\|$	Assumption on $\kappa(X)$	References
CholQR	$O(\varepsilon)\kappa^2(X)$	$O(\varepsilon)\kappa^2(X) < 1$	[Yamamoto, Nakatsukasa, Yanagisawa, Fukaya, 2015]
CholQR+	$O(\varepsilon)$	$O(\varepsilon)\kappa^2(X) < 1$	[Yamamoto, Nakatsukasa, Yanagisawa, Fukaya, 2015]
ShCholQR++	$O(\varepsilon)$	$O(\varepsilon)\kappa(X) < 1$	[Fukaya, Kannan, Nakatsukasa, Yamamoto, Yanagisawa, 2020]
HouseQR	$O(\varepsilon)$	none	[Wilkinson, 1965]
GivensQR	$O(\varepsilon)$	none	[Wilkinson, 1965]
TSQR	$O(\varepsilon)$	none	[Mori, Yamamoto, Zhang, 2012] [Demmel, Grigori, Hoemmen, Langou, 2012]

Block Classical Gram-Schmidt (BCGS)

Block CGS

$[\boldsymbol{\mathcal{Q}}, \mathcal{R}] = \text{BCGS}(\boldsymbol{\mathcal{X}})$

1: $[\boldsymbol{Q}_1, R_{11}] = \text{IntraOrtho}\,(\boldsymbol{X}_1)$
2: **for** $k = 1, \ldots, p-1$ **do**
3: $\quad \mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$
4: $\quad \boldsymbol{W} = \boldsymbol{X}_{k+1} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}_{1:k,k+1}$
5: $\quad [\boldsymbol{Q}_{k+1}, R_{k+1,k+1}] = \text{IntraOrtho}\,(\boldsymbol{W})$
6: **end for**
7: **return** $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

No existing proof of the loss of orthogonality in BCGS!

Conjecture: Even if our IntraOrtho has $O(\varepsilon)$ loss of orthogonality, BCGS is just as bad as CGS:
$$\|I - \bar{\mathcal{Q}}^T \bar{\mathcal{Q}}\| \leq O(\varepsilon)\kappa^{n-1}(\mathcal{X})$$

"Glued" matrices from [Smoktunowicz, Barlow, Langou, 2006]
$m = 1000, p = 50, s = 4$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGS ∘ HouseQR
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$

GluedBlockKappaPlot([1000 50 4], 1:8, {'BCGS'}, {'HouseQR'})

"Glued" matrices from [Smoktunowicz, Barlow, Langou, 2006]
$$m = 1000, p = 50, s = 4$$

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Legend:
- BCGS ∘ HouseQR
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x-axis: $\kappa(\mathcal{X})$
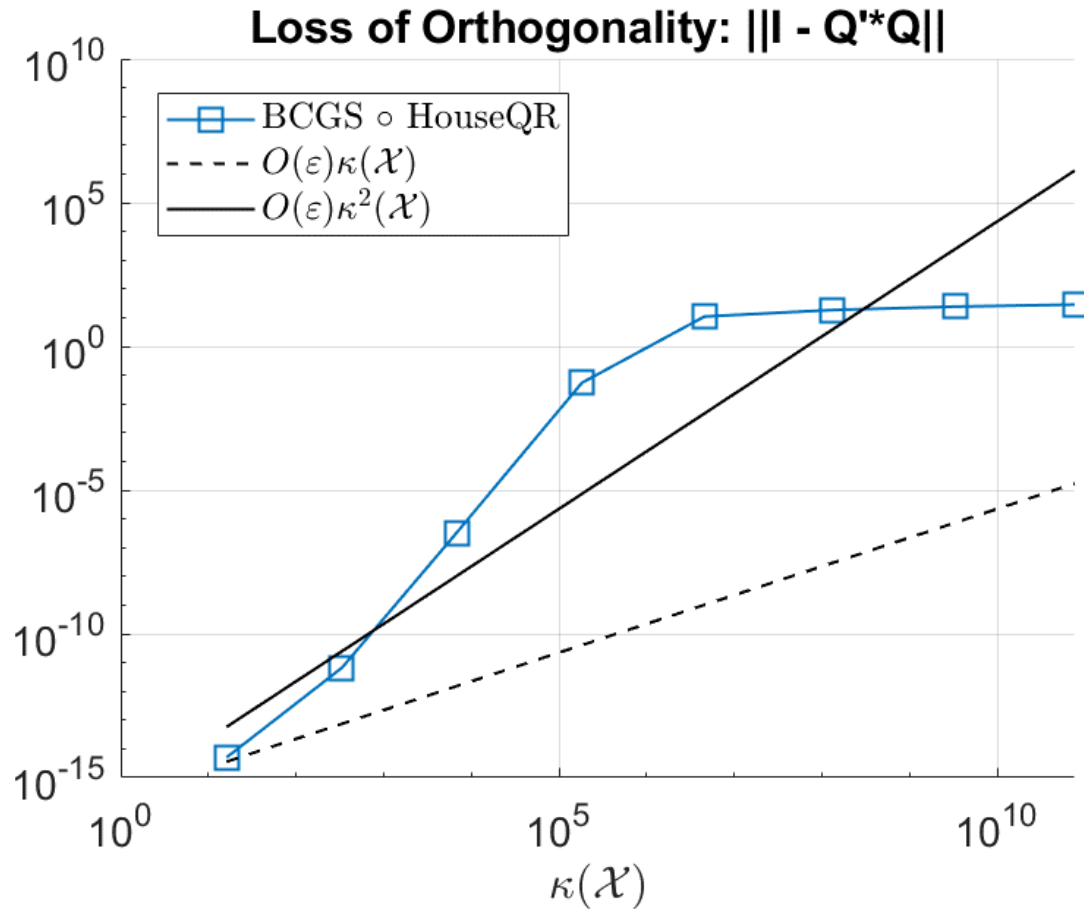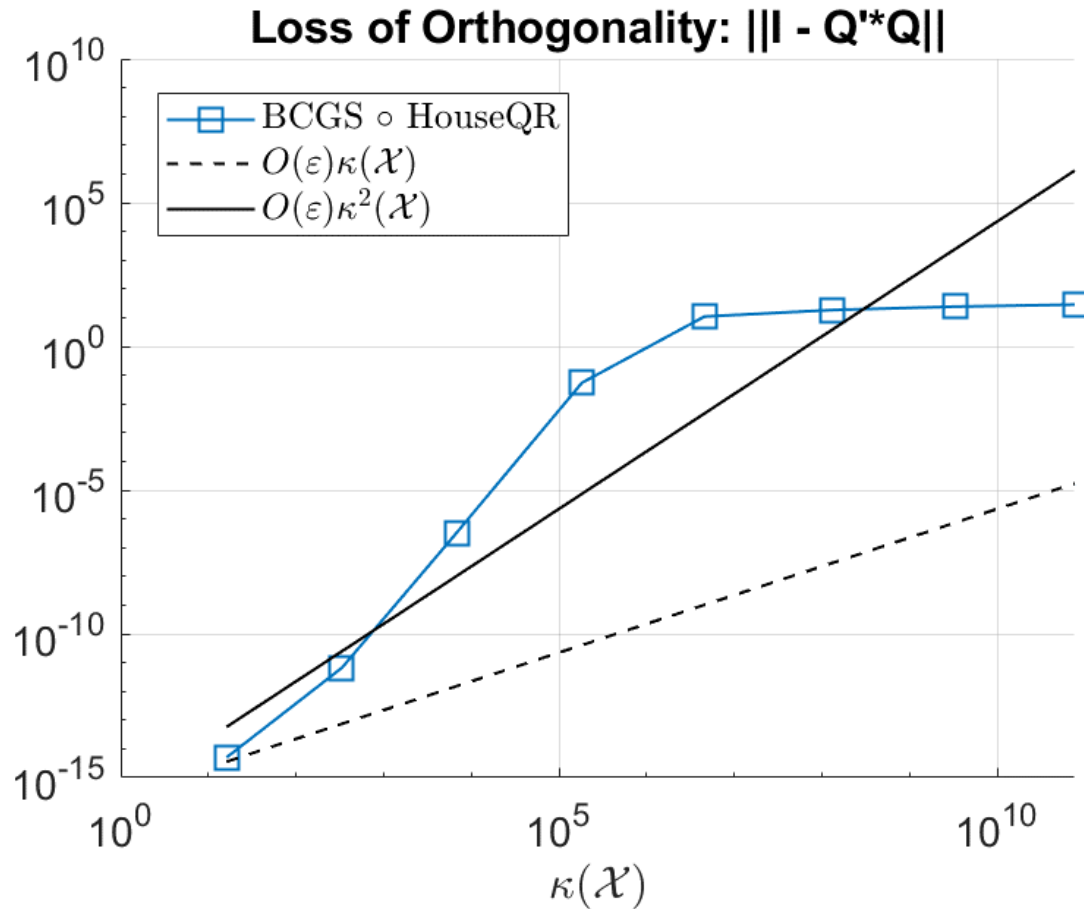
BCGS loss of orthogonality is **_not_** $O(\varepsilon)\kappa^2(\mathcal{X})$!

GluedBlockKappaPlot([1000 50 4], 1:8, {'BCGS'}, {'HouseQR'})

Block Pythagorean Theorem

Let $X, Y, Z \in \mathbb{R}^{n \times s}$ be such that $X = Y + Z$ and $Y \perp Z$. Then

$$X^T X = Y^T Y + Z^T Z.$$

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Let $X, Y, Z \in \mathbb{R}^{n \times s}$ be such that $X = Y + Z$ and $Y \perp Z$. Then

$$X^T X = Y^T Y + Z^T Z.$$

If $X = QR$, $Y = US$, and $Z = VT$ are economic QR factorizations, then

$$X^T X = Y^T Y + Z^T Z \quad = \quad R^T R = S^T S + T^T T$$

In particular,

$$S = \mathrm{chol}(Y^T Y) = \mathrm{chol}(X^T X - Z^T Z) = \mathrm{chol}(R^T R - T^T T)$$

Block Pythagorean CGS

$$W_{k+1} = X_{k+1} - \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1}$$

$$\left[Q_{k+1}, R_{k+1,k+1}\right] = \text{IntraOrtho}(W_{k+1})$$

$[\mathcal{Q}, \mathcal{R}] = \text{BCGS}(\mathcal{X})$

1: $[\boldsymbol{Q}_1, R_{11}] = \text{IntraOrtho}(\boldsymbol{X}_1)$
2: **for** $k = 1, \ldots, p-1$ **do**
3: $\quad \mathcal{R}_{1:k,k+1} = \mathcal{Q}_{1:k}^T \boldsymbol{X}_{k+1}$
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$$X_{k+1} = \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1} + W_{k+1}$$

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6: **end for**
7: **return** $\mathcal{Q} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

Let $\mathcal{R}_{1:k,k+1} = Q_\mathcal{R} P_{k+1}$ be the QR factorization of $\mathcal{R}_{1:k,k+1}$

Let $X_{k+1} = Q_X T_{k+1}$ be the QR factorization of X_{k+1}

$$T_{k+1}^T T_{k+1} = X_{k+1}^T X_{k+1}$$
$$= W_{k+1}^T W_{k+1} + \mathcal{R}_{1:k,k+1}^T \mathcal{R}_{1:k,k+1}$$
$$= R_{k+1,k+1}^T R_{k+1,k+1} + P_{k+1}^T P_{k+1}$$

Block Pythagorean CGS

$$W_{k+1} = X_{k+1} - \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1}$$

$$[Q_{k+1}, R_{k+1,k+1}] = \text{IntraOrtho}(W_{k+1})$$

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$$\begin{aligned} T_{k+1}^T T_{k+1} &= X_{k+1}^T X_{k+1} \\ &= W_{k+1}^T W_{k+1} + \mathcal{R}_{1:k,k+1}^T \mathcal{R}_{1:k,k+1} \\ &= R_{k+1,k+1}^T R_{k+1,k+1} + P_{k+1}^T P_{k+1} \end{aligned}$$

$$R_{k+1,k+1} = \text{chol}\big(X_{k+1}^T X_{k+1} - \mathcal{R}_{1:k,k+1}^T \mathcal{R}_{1:k,k+1}\big) = \text{chol}\big(T_{k+1}^T T_{k+1} - P_{k+1}^T P_{k+1}\big)$$

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Block Pythagorean CGS

$$W_{k+1} = X_{k+1} - \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1}$$

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$$X_{k+1} = \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1} + W_{k+1}$$

$[\mathcal{Q}, \mathcal{R}] = \text{BCGS}(\mathcal{X})$
1: $[Q_1, R_{11}] = \text{IntraOrtho}(X_1)$
2: **for** $k = 1, \ldots, p-1$ **do**
3: $\quad \mathcal{R}_{1:k,k+1} = \mathcal{Q}_{1:k}^T X_{k+1}$
4: $\quad W = X_{k+1} - \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1}$
5: $\quad [Q_{k+1}, R_{k+1,k+1}] = \text{IntraOrtho}(W)$
6: **end for**
7: **return** $\mathcal{Q} = [Q_1, \ldots, Q_p], \mathcal{R} = (R_{jk})$

Let $\mathcal{R}_{1:k,k+1} = Q_{\mathcal{R}}P_{k+1}$ be the QR factorization of $\mathcal{R}_{1:k,k+1}$

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$$T_{k+1}^T T_{k+1} = X_{k+1}^T X_{k+1}$$

$$= W_{k+1}^T W_{k+1} + \mathcal{R}_{1:k,k+1}^T \mathcal{R}_{1:k,k+1}$$

$$= R_{k+1,k+1}^T R_{k+1,k+1} + P_{k+1}^T P_{k+1}$$

$$R_{k+1,k+1} = \text{chol}\left(X_{k+1}^T X_{k+1} - \mathcal{R}_{1:k,k+1}^T \mathcal{R}_{1:k,k+1}\right) = \text{chol}\left(T_{k+1}^T T_{k+1} - P_{k+1}^T P_{k+1}\right)$$

BCGS-PIP

BCGS-PIO

BCGS-PIP and BCGS-PIO

$[\boldsymbol{\mathcal{Q}}, \mathcal{R}] = \texttt{BCGS}(\boldsymbol{\mathcal{X}})$

1: $[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$
2: **for** $k = 1, \ldots, p-1$ **do**
3:     $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$
4:     $\boldsymbol{W} = \boldsymbol{X}_{k+1} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}_{1:k,k+1}$
5:     $[\boldsymbol{Q}_{k+1}, R_{k+1,k+1}] = \texttt{IntraOrtho}\,(\boldsymbol{W})$
6: **end for**
7: **return** $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

$[\boldsymbol{\mathcal{Q}}, \mathcal{R}] = \texttt{BCGS-PIP}(\boldsymbol{\mathcal{X}})$

1: $[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$
2: **for** $k = 1, \ldots, p-1$ **do**
3:     $\begin{bmatrix} \mathcal{R}_{1:k,k+1} \\ \mathcal{Z}_{k+1} \end{bmatrix} = [\boldsymbol{\mathcal{Q}}_{1:k} \ \boldsymbol{X}_{k+1}]^T \boldsymbol{X}_{k+1}$
4:     $R_{k+1,k+1} = \texttt{chol}(\mathcal{Z}_{k+1} - \mathcal{R}_{1:k,k+1}^T \mathcal{R}_{1:k,k+1})$
5:     $\boldsymbol{W}_{k+1} = \boldsymbol{X}_{k+1} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}_{1:k,k+1}$
6:     $\boldsymbol{Q}_{k+1} = \boldsymbol{W}_{k+1} R_{k+1,k+1}^{-1}$
7: **end for**

$[\boldsymbol{\mathcal{Q}}, \mathcal{R}] = \texttt{BCGS-PIO}(\boldsymbol{\mathcal{X}})$

1: $[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$
2: **for** $k = 1, \ldots, p-1$ **do**
3:     $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$
4:     $\left[\sim, \begin{bmatrix} T_{k+1} \\ & P_{k+1} \end{bmatrix}\right] = \texttt{IntraOrtho}\left(\begin{bmatrix} \boldsymbol{X}_{k+1} \\ & \mathcal{R}_{1:k,k+1} \end{bmatrix}\right)$
5:     $R_{k+1,k+1} = \texttt{chol}(T_{k+1}^T T_{k+1} - P_{k+1}^T P_{k+1})$
6:     $\boldsymbol{W}_{k+1} = \boldsymbol{X}_{k+1} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}_{1:k,k+1}$
7:     $\boldsymbol{Q}_{k+1} = \boldsymbol{W}_{k+1} R_{k+1,k+1}^{-1}$
8: **end for**

- See [C., Lund, Rozložník, Thomas, 2020] and [C., Lund, Rozložník, 2021]
- BCGS-PIP also developed independently by [Yamazaki, Thomas, Hoemmen, Boman, Świrydowicz, Elliott, 2020]; called "CGS+CholQR"

Let $\mathcal{X} \in \mathbb{R}^{m \times n}$ be a matrix whose columns are organized into p blocks of size s, and assume that

$$O(\varepsilon)\kappa^2(\mathcal{X}) < 1.$$

Suppose we execute BCGS-PIP ∘ IntraOrtho($\mathcal{X}$) or BCGS-PIO ∘ IntraOrtho($\mathcal{X}$) on a machine with unit roundoff ε.

If for all X, IntraOrtho(X) computes factors $\bar{Q}$ and $\bar{R}$ that satisfy

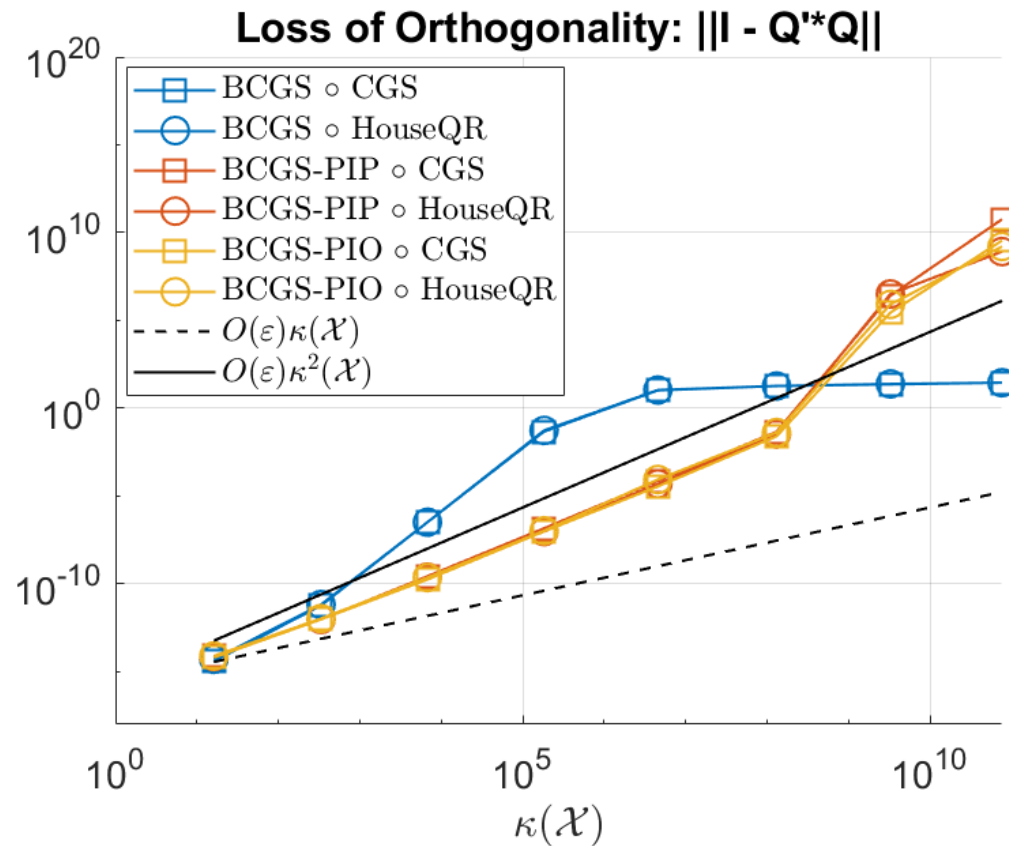$$\bar{R}^T\bar{R} = X^TX + \Delta E, \qquad \|\Delta E\| \le O(\varepsilon)\|X\|^2, \quad \text{and}$$
$$\bar{Q}\bar{R} = X + \Delta D, \qquad \|\Delta D\| \le O(\varepsilon)(\|X\| + \|\bar{Q}\|\|\bar{R}\|),$$

then the factors $\bar{\mathcal{Q}}$ and $\bar{\mathcal{R}}$ satisfy

$$\|I - \bar{\mathcal{Q}}^T\bar{\mathcal{Q}}\| \le O(\varepsilon)\kappa^2(\mathcal{X}), \qquad \text{and}$$
$$\bar{\mathcal{Q}}\bar{\mathcal{R}} = \mathcal{X} + \Delta\mathcal{D}, \qquad \|\Delta\mathcal{D}\| \le O(\varepsilon)\|\mathcal{X}\|.$$

[C., Lund, Rozložník, 2021] 28

"Glued" matrices from [Smoktunowicz, Barlow, Langou, 2006]
$$m = 1000, p = 50, s = 4$$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGS ∘ CGS
- BCGS ∘ HouseQR
- BCGS-PIP ∘ CGS
- BCGS-PIP ∘ HouseQR
- BCGS-PIO ∘ CGS
- BCGS-PIO ∘ HouseQR
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$

Summary: BCGS Variants

Algorithm	$\|I - \bar{Q}^T \bar{Q}\|$	Assumption on $\kappa(\mathcal{X})$	References
BCGS	$O(\varepsilon)\kappa^{n-1}(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	conjecture
BCGS-P	$O(\varepsilon)\kappa^2(\mathcal{X})$	$O(\varepsilon)\kappa^2(\mathcal{X}) < 1$	[C., Lund, Rozložník, 2021]

Reorthogonalized Block Gram-Schmidt Variants

BCGSI+

[Barlow and Smoktunowicz, 2013]: If we have an IntraOrtho with $\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)$ and if $O(\varepsilon)\kappa(\mathcal{X}) < 1$, then for BCGSI+,

$$\|I - \bar{\mathcal{Q}}^T \bar{\mathcal{Q}}\| \leq O(\varepsilon).$$

$[\mathcal{Q}, \mathcal{R}] = \texttt{BCGSI+}(\mathcal{X})$

1: Allocate memory for $\mathcal{Q}$ and $\mathcal{R}$
2: $[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$
3: **for** $k = 1, \ldots, p - 1$ **do**
4: $\quad \mathcal{R}^{(1)}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}^T_{1:k} \boldsymbol{X}_{k+1}$ % first BCGS step
5: $\quad \boldsymbol{W} = \boldsymbol{X}_{k+1} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}^{(1)}_{1:k,k+1}$
6: $\quad [\widehat{\boldsymbol{Q}}, R^{(1)}_{k+1,k+1}] = \texttt{IntraOrtho}\,(\boldsymbol{W})$
7: $\quad \mathcal{R}^{(2)}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}^T_{1:k} \widehat{\boldsymbol{Q}}$ % second BCGS step
8: $\quad \boldsymbol{W} = \widehat{\boldsymbol{Q}} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}^{(2)}_{1:k,k+1}$
9: $\quad [\boldsymbol{Q}_{k+1}, R^{(2)}_{k+1,k+1}] = \texttt{IntraOrtho}\,(\boldsymbol{W})$
10: $\quad \mathcal{R}_{1:k,k+1} = \mathcal{R}^{(1)}_{1:k,k+1} + \mathcal{R}^{(2)}_{1:k,k+1} R^{(1)}_{k+1,k+1}$
11: $\quad R_{k+1,k+1} = R^{(2)}_{k+1,k+1} R^{(1)}_{k+1,k+1}$
12: **end for**
13: **return** $\mathcal{Q} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p], \mathcal{R} = (R_{jk})$

BCGSI+

[Barlow and Smoktunowicz, 2013]: If we have an IntraOrtho with $\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)$ and if $O(\varepsilon)\kappa(\mathcal{X}) < 1$, then for BCGSI+,

$$\|I - \bar{\mathcal{Q}}^T \bar{\mathcal{Q}}\| \leq O(\varepsilon).$$

Key approach: Obtain bounds for the subproblem in every step of BCGSI+:

Given a near left-orthogonal matrix $\mathcal{U} \in \mathbb{R}^{m \times t}$ and a matrix $B \in \mathbb{R}^{m \times s}$, find $S \in \mathbb{R}^{t \times s}$, upper triangular $R_B \in \mathbb{R}^{s \times s}$, and left-orthogonal Q such that

$$B = \mathcal{U}S + QR_B \quad \text{and} \quad \mathcal{U}^T Q \approx 0.$$

*Requires the a priori assumption that $O(\varepsilon)\|B\|\|\bar{R}_B^{-1}\| < 1$

$$[\mathcal{Q}, \mathcal{R}] = \texttt{BCGSI+}(\mathcal{X})$$

1: Allocate memory for $\mathcal{Q}$ and $\mathcal{R}$
2: $[Q_1, R_{11}] = \texttt{IntraOrtho}(X_1)$
3: **for** $k = 1, \ldots, p-1$ **do**
4:    $\mathcal{R}^{(1)}_{1:k,k+1} = \mathcal{Q}^T_{1:k} X_{k+1}$ % first BCGS step
5:    $W = X_{k+1} - \mathcal{Q}_{1:k} \mathcal{R}^{(1)}_{1:k,k+1}$
6:    $[\widehat{Q}, R^{(1)}_{k+1,k+1}] = \texttt{IntraOrtho}(W)$
7:    $\mathcal{R}^{(2)}_{1:k,k+1} = \mathcal{Q}^T_{1:k}\widehat{Q}$ % second BCGS step
8:    $W = \widehat{Q} - \mathcal{Q}_{1:k}\mathcal{R}^{(2)}_{1:k,k+1}$
9:    $[Q_{k+1}, R^{(2)}_{k+1,k+1}] = \texttt{IntraOrtho}(W)$
10:    $\mathcal{R}_{1:k,k+1} = \mathcal{R}^{(1)}_{1:k,k+1} + \mathcal{R}^{(2)}_{1:k,k+1}R^{(1)}_{k+1,k+1}$
11:    $R_{k+1,k+1} = R^{(2)}_{k+1,k+1}R^{(1)}_{k+1,k+1}$
12: **end for**
13: **return** $\mathcal{Q} = [Q_1, \ldots, Q_p], \mathcal{R} = (R_{jk})$

BCGSI+

[Barlow and Smoktunowicz, 2013]: If we have an IntraOrtho with $\|I - \bar{Q}^T\bar{Q}\| \le O(\varepsilon)$ and if $O(\varepsilon)\kappa(\mathcal{X}) < 1$, then for BCGSI+,

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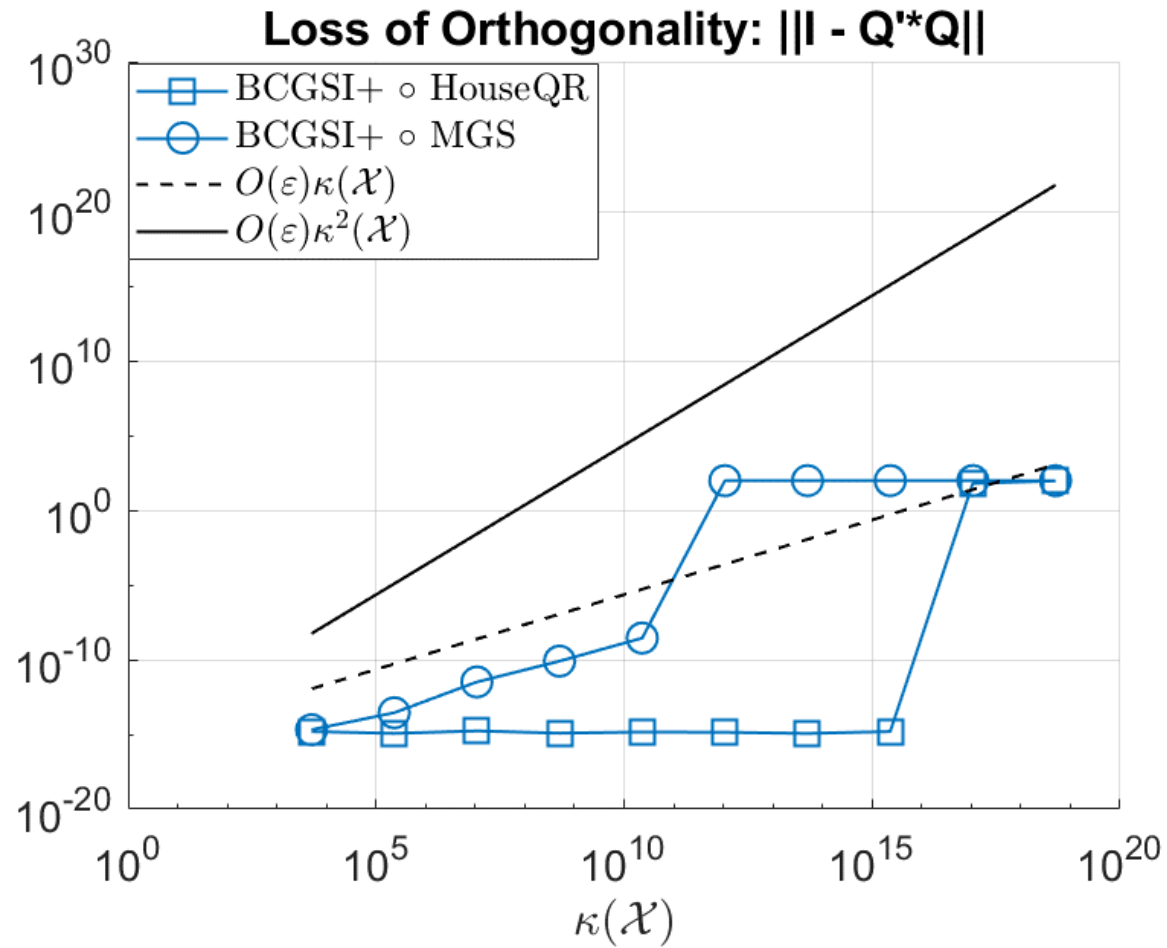
$$B = \mathcal{U}S + QR_B \quad \text{and} \quad \mathcal{U}^T Q \approx 0.$$

$[\mathcal{Q}, \mathcal{R}] = \texttt{BCGSI+}(\mathcal{X})$
1: Allocate memory for $\mathcal{Q}$ and $\mathcal{R}$
2: $[Q_1, R_{11}] = \texttt{IntraOrtho}(X_1)$
3: **for** $k = 1, \ldots, p-1$ **do**
4:    $\mathcal{R}^{(1)}_{1:k,k+1} = \mathcal{Q}^T_{1:k}X_{k+1}$ % first BCGS step
5:    $W = X_{k+1} - \mathcal{Q}_{1:k}\mathcal{R}^{(1)}_{1:k,k+1}$
6:    $[\widehat{Q}, R^{(1)}_{k+1,k+1}] = \texttt{IntraOrtho}(W)$
7:    $\mathcal{R}^{(2)}_{1:k,k+1} = \mathcal{Q}^T_{1:k}\widehat{Q}$ % second BCGS step
8:    $W = \widehat{Q} - \mathcal{Q}_{1:k}\mathcal{R}^{(2)}_{1:k,k+1}$
9:    $[Q_{k+1}, R^{(2)}_{k+1,k+1}] = \texttt{IntraOrtho}(W)$
10:    $\mathcal{R}_{1:k,k+1} = \mathcal{R}^{(1)}_{1:k,k+1} + \mathcal{R}^{(2)}_{1:k,k+1}R^{(1)}_{k+1,k+1}$
11:    $R_{k+1,k+1} = R^{(2)}_{k+1,k+1}R^{(1)}_{k+1,k+1}$
12: **end for**
13: **return** $\mathcal{Q} = [Q_1, \ldots, Q_p], \mathcal{R} = (R_{jk})$

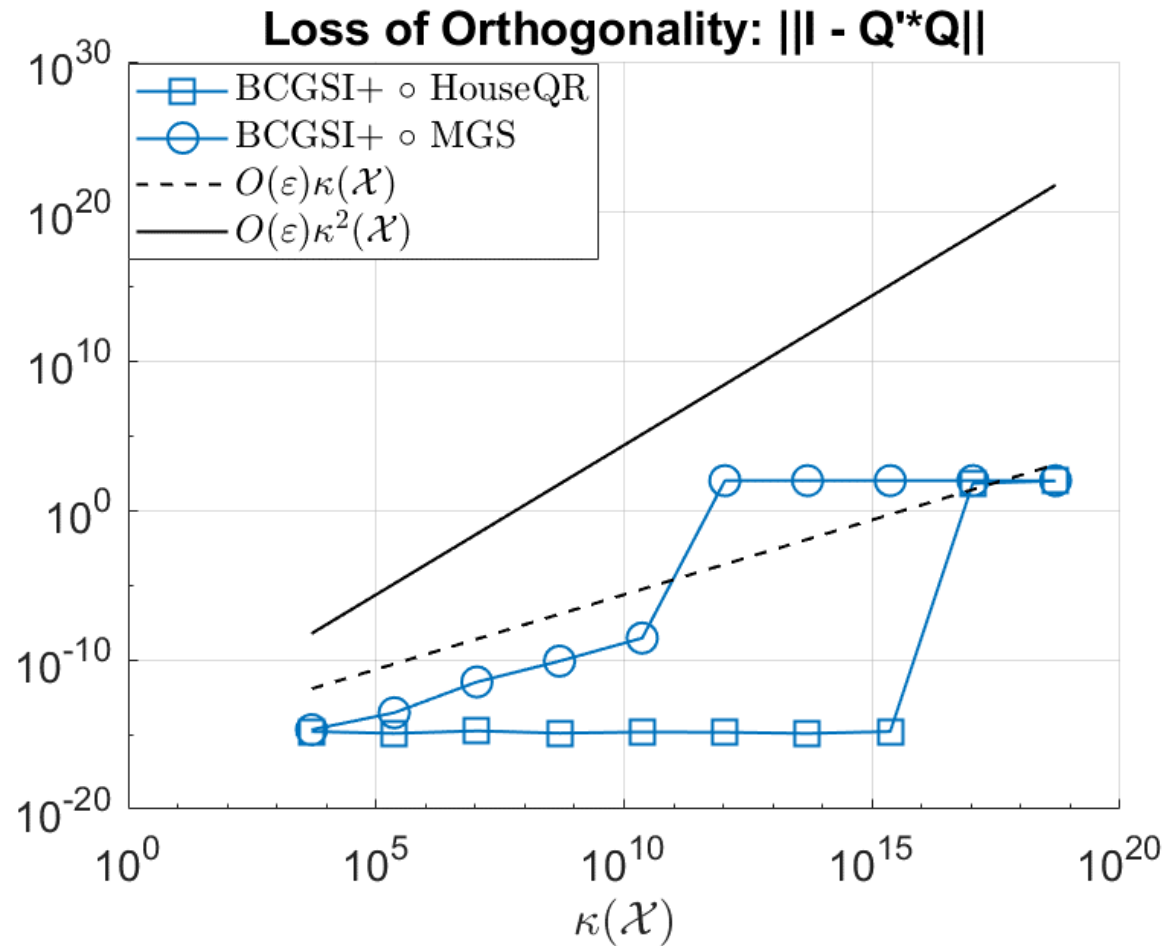*Requires the a priori assumption that $O(\varepsilon)\|B\|\|\bar{R}_B^{-1}\| < 1$

*The requirement that *IntraOrtho has $\|I - \bar{Q}^T\bar{Q}\| \le O(\varepsilon)$ is needed to guarantee that Q_1 is near left-orthogonal*; proof proceeds via induction.

Läuchli matrix
$m = 1000, p = 100, s = 5$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGSI+ ∘ HouseQR (squares)
- BCGSI+ ∘ MGS (circles)
- $O(\varepsilon)\kappa(\mathcal{X})$ (dashed)
- $O(\varepsilon)\kappa^2(\mathcal{X})$ (solid)

x-axis: $\kappa(\mathcal{X})$

```
LaeuchliBlockKappaPlot([1000 100 5],  logspace(-1, -16, 10), {'BCGS_IRO'}, {'HouseQR','MGS'})
```

Läuchli matrix
$$m = 1000, p = 100, s = 5$$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGSI+ ∘ HouseQR
- BCGSI+ ∘ MGS
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$

Recall: need $\left\| I - \bar{Q}_1^T \bar{Q}_1 \right\| \leq O(\varepsilon)$ to satisfy base case

⇒ Idea: What if we use a less stable IntraOrtho and just reorthogonalize the first block Q_1?

`LaeuchliBlockKappaPlot([1000 100 5], logspace(-1, -16, 10), {'BCGS_IRO'}, {'HouseQR','MGS'})`

Läuchli matrix
$m = 1000, p = 100, s = 5$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGSI+ ∘ HouseQR
- BCGSI+ ∘ MGS
- BCGSI+1 ∘ MGS
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$
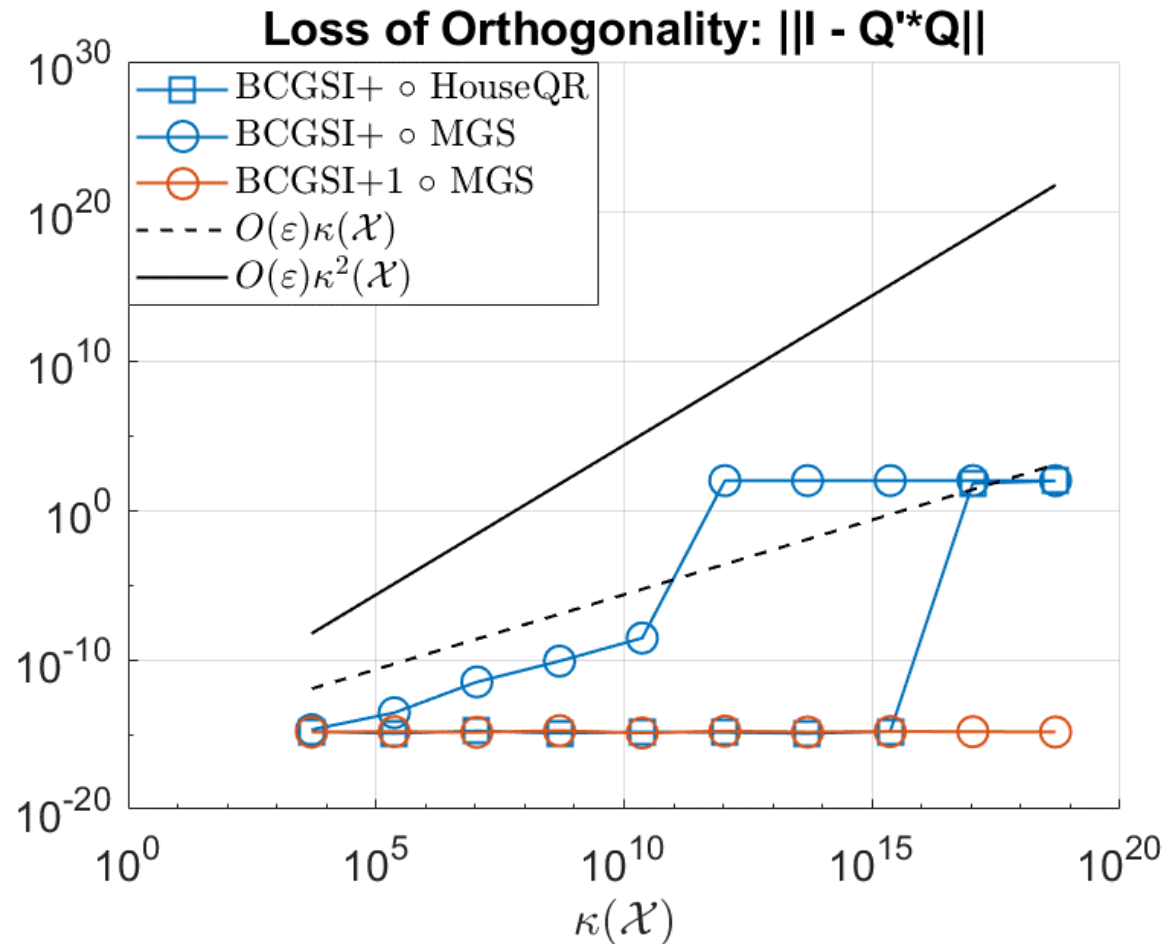
BCGSI+1 [C., Lund, Rozložník, Thomas]:
Reorthogonalization on the first block to ensure $\left\| I - \bar{Q}_1^T \bar{Q}_1 \right\| \le O(\varepsilon)$

`LaeuchliBlockKappaPlot([1000 100 5],  logspace(-1, -16, 10), {'BCGS_IRO','BCGS_IRO_1'}, {'HouseQR','MGS'})`

BCGSI+LS

- Block generalization of CGSI+LS

- Equivalent algorithm given in [Yamazaki, Thomas, Hoemmen, Boman, Świrydowicz, Elliott, 2020] (see Figure 3)

- Notice: no IntraOrtho

- Conjectured that CGSI+LS has $O(\varepsilon)$ loss of orthogonality
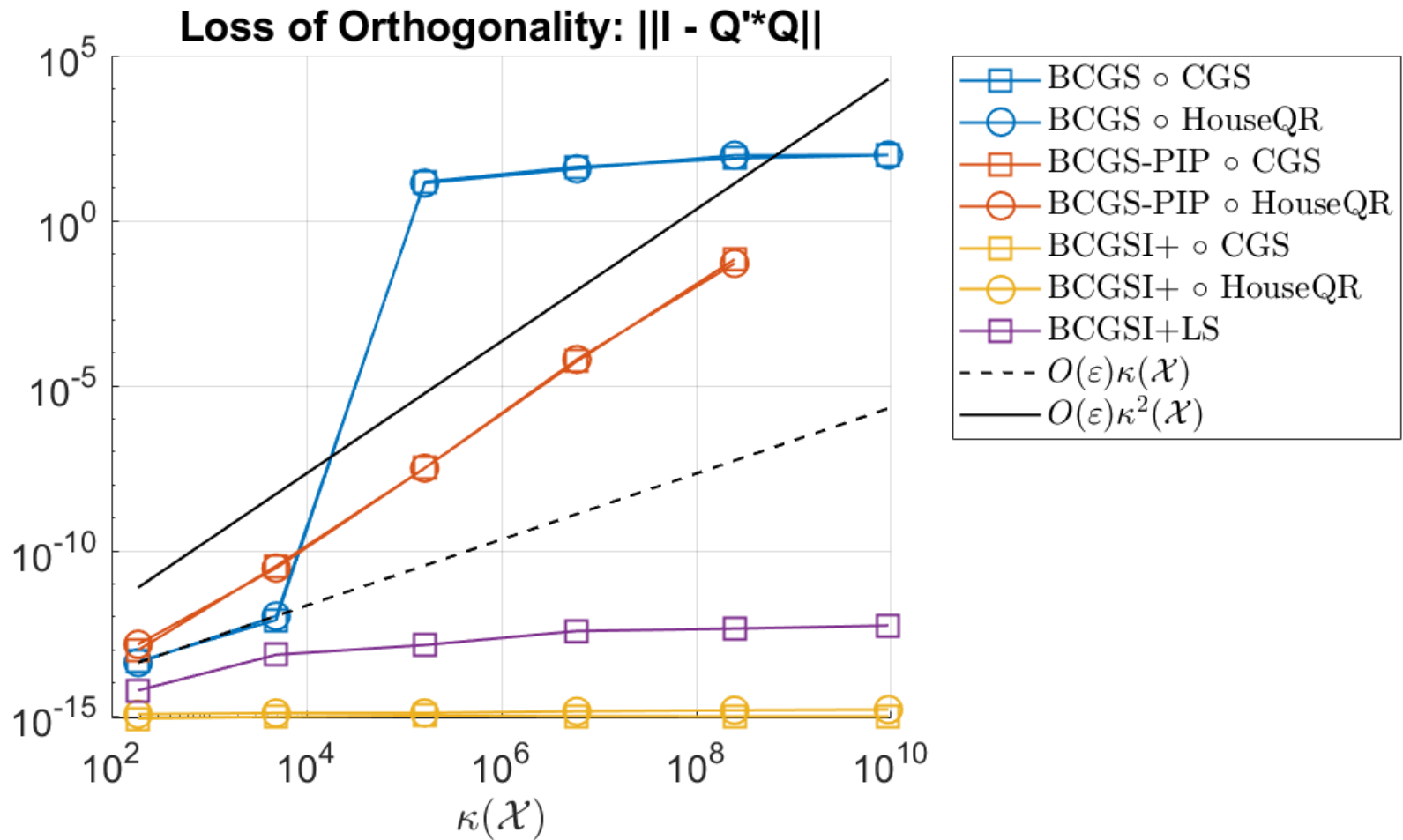 - What about BCGSI+LS?

$[\boldsymbol{\mathcal{Q}}, \mathcal{R}] = \texttt{BCGSI+LS}(\boldsymbol{\mathcal{X}})$

1: Allocate memory for $\boldsymbol{\mathcal{Q}}$ and $\mathcal{R}$
2: $\boldsymbol{U} = \boldsymbol{X}_1$
3: **for** $k = 2, \ldots p$ **do**
4:     **if** $k = 2$ **then**
5:        $[R_{k-1,k-1}^T R_{k-1,k-1} \; P] = \boldsymbol{U}^T[\boldsymbol{U} \; \boldsymbol{X}_k]$
6:     **else if** $k > 2$ **then**
7:        $\begin{bmatrix} \boldsymbol{W} & \boldsymbol{Z} \\ \Omega & Z \end{bmatrix} = [\boldsymbol{\mathcal{Q}}_{1:k-2} \; \boldsymbol{U}]^T[\boldsymbol{U} \; \boldsymbol{X}_k]$
8:        $[R_{k-1,k-1}^T R_{k-1,k-1} \; P] = [\Omega \; Z] - \boldsymbol{W}^T[\boldsymbol{W} \; \boldsymbol{Z}]$
9:     **end if**
10:    $R_{k-1,k} = R_{k-1,k-1}^{-T} P$
11:    **if** $k = 2$ **then**
12:       $\boldsymbol{Q}_{k-1} = \boldsymbol{U} R_{k-1,k-1}^{-1}$
13:    **else if** $k > 2$ **then**
14:       $\mathcal{R}_{1:k-2,k-1} = \mathcal{R}_{1:k-2,k-1} + \boldsymbol{W}$
15:       $\mathcal{R}_{1:k-2,k} = \boldsymbol{Z}$
16:       $\boldsymbol{Q}_{k-1} = (\boldsymbol{U} - \boldsymbol{\mathcal{Q}}_{1:k-2}\boldsymbol{W})R_{k-1,k-1}^{-1}$
17:    **end if**
18:    $\boldsymbol{U} = \boldsymbol{X}_k - \boldsymbol{\mathcal{Q}}_{1:k-1}\mathcal{R}_{1:k-1,k}$
19: **end for**
20: $\begin{bmatrix} \boldsymbol{W} \\ \Omega \end{bmatrix} = [\boldsymbol{\mathcal{Q}}_{1:s-1} \; \boldsymbol{U}]^T \boldsymbol{U}$
21: $R_{s,s}^T R_{s,s} = \Omega - \boldsymbol{W}^T \boldsymbol{W}$
22: $\mathcal{R}_{1:s-1,s} = \mathcal{R}_{1:s-1,s} + \boldsymbol{W}$
23: $\boldsymbol{Q}_s = (\boldsymbol{U} - \boldsymbol{\mathcal{Q}}_{1:s-1}\boldsymbol{W})R_{s,s}^{-1}$
24: **return** $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_s]$, $\mathcal{R} = (R_{jk})$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGS ∘ CGS
- BCGS ∘ HouseQR
- BCGS-PIP ∘ CGS
- BCGS-PIP ∘ HouseQR
- BCGSI+ ∘ CGS
- BCGSI+ ∘ HouseQR
- BCGSI+LS
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

"Monomial" matrices: Each block $X_k = [v_k, Av_k, \ldots, A^{s-1}v_k]$, where A is a diagonal $m \times m$ matrix with uniformly distributed eigenvalues in (.1,10) and v_k random

MonomialBlockKappaPlot([1000 120 2], 2:2:12, {'BCGS', 'BCGS_PIP','BCGS_IRO', 'BCGS_IRO_LS'}, {'CGS', 'HouseQR'})

Summary: BCGS Variants

Algorithm	$\|I - \bar{Q}^T \bar{Q}\|$	Assumption on $\kappa(\mathcal{X})$	References
BCGS	$O(\varepsilon)\kappa^{n-1}(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	conjecture
BCGS-P	$O(\varepsilon)\kappa^2(\mathcal{X})$	$O(\varepsilon)\kappa^2(\mathcal{X}) < 1$	[C., Lund, Rozložník, 2021]
BCGSI+	$O(\varepsilon)$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	[Barlow and Smoktunowicz, 2013]
BCGSI+1	$O(\varepsilon)$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	conjecture
BCGSS+rpl	$O(\varepsilon)$	none	conjecture, [Stewart, 2008]
BCGSI+LS	?	?	

Block Modified Gram-Schmidt (BMGS)

Intuition: From lines 4-8:

$$W = \left(I - Q_k Q_k^T\right) \cdots \left(I - Q_1 Q_1^T\right) X_{k+1}$$

Each projector $I - Q_j Q_j^T$ is equivalent to a step of CGS

- $\Rightarrow$ Underlying "CGS-like" nature of BMGS

$[\mathcal{Q}, \mathcal{R}] = \text{BMGS}(\mathcal{X})$

1: Allocate memory for $\mathcal{Q}$ and $\mathcal{R}$
2: $[Q_1, R_{11}] = \text{IntraOrtho}(X_1)$
3: **for** $k = 1, \ldots, p-1$ **do**
4: $\quad W = X_{k+1}$
5: $\quad$ **for** $j = 1, \ldots, k$ **do**
6: $\quad\quad R_{j,k+1} = Q_j^T W$
7: $\quad\quad W = W - Q_j R_{j,k+1}$
8: $\quad$ **end for**
9: $\quad [Q_{k+1}, R_{k+1,k+1}] = \text{IntraOrtho}(W)$
10: **end for**
11: **return** $\mathcal{Q} = [Q_1, \ldots, Q_p]$, $\mathcal{R} = (R_{jk})$

Results of Jalby and Philippe (1991)

Intuition: From lines 4-8:

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- $\Rightarrow$ Underlying "CGS-like" nature of BMGS

[Jalby and Philippe, 1991]:

- BMGS∘MGS behaves "like CGS"

- BMGS∘MGS+ is as stable as MGS

$[\mathcal{Q}, \mathcal{R}] = \texttt{BMGS}(\boldsymbol{\mathcal{X}})$

1: Allocate memory for $\mathcal{Q}$ and $\mathcal{R}$
2: $[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}(\boldsymbol{X}_1)$
3: **for** $k = 1, \ldots, p-1$ **do**
4:     $\boldsymbol{W} = \boldsymbol{X}_{k+1}$
5:     **for** $j = 1, \ldots, k$ **do**
6:         $R_{j,k+1} = \boldsymbol{Q}_j^T \boldsymbol{W}$
7:         $\boldsymbol{W} = \boldsymbol{W} - \boldsymbol{Q}_j R_{j,k+1}$
8:     **end for**
9:     $[\boldsymbol{Q}_{k+1}, R_{k+1,k+1}] = \texttt{IntraOrtho}(\boldsymbol{W})$
10: **end for**
11: **return** $\mathcal{Q} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p], \mathcal{R} = (R_{jk})$

Results of Jalby and Philippe (1991)

Intuition: From lines 4-8:

$$W = \left(I - Q_k Q_k^T\right) \cdots \left(I - Q_1 Q_1^T\right) X_{k+1}$$

Each projector $I - Q_j Q_j^T$ is equivalent to a step of CGS

- $\Rightarrow$ Underlying "CGS-like" nature of BMGS

[Jalby and Philippe, 1991]:

- BMGS∘MGS behaves "like CGS"

- BMGS∘MGS+ is as stable as MGS

- Can manipulate proof of Theorem 4.1 from Jalby and Philippe's work to show that BMGS ∘ (any IntraOrtho with $\|I - \bar{Q}^T \bar{Q}\| \le O(\varepsilon)$) is as stable as MGS

$[\mathcal{Q}, \mathcal{R}] = \text{BMGS}(\boldsymbol{\mathcal{X}})$

1: Allocate memory for $\mathcal{Q}$ and $\mathcal{R}$
2: $[\boldsymbol{Q}_1, R_{11}] = \text{IntraOrtho}(\boldsymbol{X}_1)$
3: **for** $k = 1, \ldots, p-1$ **do**
4:    $\boldsymbol{W} = \boldsymbol{X}_{k+1}$
5:    **for** $j = 1, \ldots, k$ **do**
6:       $R_{j,k+1} = \boldsymbol{Q}_j^T \boldsymbol{W}$
7:       $\boldsymbol{W} = \boldsymbol{W} - \boldsymbol{Q}_j R_{j,k+1}$
8:    **end for**
9:    $[\boldsymbol{Q}_{k+1}, R_{k+1,k+1}] = \text{IntraOrtho}(\boldsymbol{W})$
10: **end for**
11: **return** $\mathcal{Q} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p], \mathcal{R} = (R_{jk})$

Block Low-Sync Variants

	Two synchronizations	One synchronization
$(I - Q_k T_k^T Q_k^T)x_{k+1}$ (matrix-matrix multiplication)	MGS-SVL [Barlow, 2019] (called "MGS2")	MGS-CWY [Świrydowicz et al., 2020]
$(I - Q_k T_k^{-T} Q_k^T)x_{k+1}$ (triangular solve)	MGS-LTS [Świrydowicz et al., 2020]	MGS-ICWY [Świrydowicz et al., 2020]

Block generalizations:

- BMGS-SVL∘MGS-SVL [Barlow, 2019] (called "MGS3")
- BMGS-SVL∘HouseQR [Barlow, 2019] (called "BMGS_H")
- BMGS-LTS: [C. Lund, Rozložník, Thomas, 2020]
- BMGS-CWY, BMGS-ICWY ([C. Lund, Rozložník, Thomas, 2020] and [Yamazaki et al., 2020])

Key quantities:

$$\Delta_{\mathcal{TS}} = \bar{\mathcal{T}}\mathcal{S} - I$$
$$\Delta_{\bar{\mathcal{Q}}\bar{\mathcal{R}}} = \bar{\mathcal{Q}}\bar{\mathcal{R}} - \mathcal{X}$$
$$\Gamma_{\mathcal{TR}} = (I - \bar{\mathcal{T}})\bar{\mathcal{R}}$$

$\mathcal{S} = \mathrm{triu}(\bar{\mathcal{Q}}^T\bar{\mathcal{Q}})$, and in exact arithmetic, $\mathcal{S} = \mathcal{T}^{-1}$.

Key quantities:

$$\Delta_{\mathcal{TS}} = \bar{\mathcal{T}}\mathcal{S} - I$$
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$$\Gamma_{\mathcal{TR}} = (I - \bar{\mathcal{T}})\bar{\mathcal{R}}$$

$\mathcal{S} = \text{triu}(\bar{\mathcal{Q}}^T\bar{\mathcal{Q}})$, and in exact arithmetic, $\mathcal{S} = \mathcal{T}^{-1}$.

[Barlow, 2019]: If $[\bar{Q}, \bar{R}, \bar{T}] = \text{IntraOrtho}(X)$ satisfies

$$\Delta_{TS} = \bar{T}S - I_s, \quad \|\Delta_{TS}\|_F \leq O(\varepsilon)$$
$$\Delta_{\bar{Q}\bar{R}} = \bar{Q}\bar{R} - X, \quad \|\Delta_{\bar{Q}\bar{R}}\|_F \leq O(\varepsilon)\|X\|_F$$
$$\Gamma_{TR} = (I - \bar{T})\bar{R}, \quad \|\Gamma_{TR}\|_F \leq O(\varepsilon)\|X\|_F$$

Then BMGS-SVL ∘ IntraOrtho($\mathcal{X}$) satisfies

$$\|\Delta_{\mathcal{TS}}\|_F \leq O(\varepsilon)$$
$$\|\Delta_{\bar{\mathcal{Q}}\bar{\mathcal{R}}}\|_F \leq O(\varepsilon)\|\mathcal{X}\|_F$$
$$\|\Gamma_{\mathcal{TR}}\|_F \leq O(\varepsilon)\|\mathcal{X}\|_F$$

Key quantities:

$$\Delta_{\mathcal{TS}} = \bar{\mathcal{T}}\mathcal{S} - I$$
$$\Delta_{\bar{\mathcal{Q}}\bar{\mathcal{R}}} = \bar{\mathcal{Q}}\bar{\mathcal{R}} - \mathcal{X}$$
$$\Gamma_{\mathcal{TR}} = (I - \bar{\mathcal{T}})\bar{\mathcal{R}}$$

$\mathcal{S} = \text{triu}(\bar{\mathcal{Q}}^T\bar{\mathcal{Q}})$, and in exact arithmetic, $\mathcal{S} = \mathcal{T}^{-1}$.

[Barlow, 2019]: If $[\bar{Q}, \bar{R}, \bar{T}] = \text{IntraOrtho}(X)$ satisfies

$$\Delta_{TS} = \bar{T}S - I_s, \quad \|\Delta_{TS}\|_F \leq O(\varepsilon)$$
$$\Delta_{\bar{Q}\bar{R}} = \bar{Q}\bar{R} - X, \quad \|\Delta_{\bar{Q}\bar{R}}\|_F \leq O(\varepsilon)\|X\|_F$$
$$\Gamma_{TR} = (I - \bar{T})\bar{R}, \quad \|\Gamma_{TR}\|_F \leq O(\varepsilon)\|X\|_F$$

Then BMGS-SVL ∘ IntraOrtho($\mathcal{X}$) satisfies

$$\|\Delta_{\mathcal{TS}}\|_F \leq O(\varepsilon)$$
$$\|\Delta_{\bar{\mathcal{Q}}\bar{\mathcal{R}}}\|_F \leq O(\varepsilon)\|\mathcal{X}\|_F$$
$$\|\Gamma_{\mathcal{TR}}\|_F \leq O(\varepsilon)\|\mathcal{X}\|_F$$

$$\|I - \bar{\mathcal{Q}}^T\bar{\mathcal{Q}}\|_F \leq O(\varepsilon)\kappa(\mathcal{X})$$
$$\text{if } O(\varepsilon)\kappa(\mathcal{X}) < 1$$

Barlow proves directly that MGS-SVL satisfies the IntraOrtho constraints

- What about BMGS-SVL with IntraOrthos that don't produce T's?

Barlow's Analysis [2019]

- What about BMGS-SVL with IntraOrthos that don't produce T's?

- Implicitly, they produce $\bar{T} = I$

- In this case,

$$\|\Delta_{TS}\|_F = \|\bar{T}S - I\|_F = \|\mathrm{I} - \mathrm{triu}(\bar{Q}^T\bar{Q})\|_F \leq \|I - \bar{Q}^T\bar{Q}\|_F$$

$$\left\|\Delta_{\bar{Q}\bar{R}}\right\|_F = \|\bar{Q}\bar{R} - X\|_F$$

$$\|\Gamma_{TR}\|_F = \|(I - \bar{T})\bar{R}\|_F = 0$$

Barlow's Analysis [2019]

- What about BMGS-SVL with IntraOrthos that don't produce T's?

- Implicitly, they produce $\bar{T} = I$

- In this case,

$$\|\Delta_{TS}\|_F = \|\bar{T}S - I\|_F = \|\mathrm{I} - \mathrm{triu}(\bar{Q}^T \bar{Q})\|_F \leq \|I - \bar{Q}^T \bar{Q}\|_F$$

$$\left\|\Delta_{\bar{Q}\bar{R}}\right\|_F = \|\bar{Q}\bar{R} - X\|_F$$

$$\|\Gamma_{TR}\|_F = \|(I - \bar{T})\bar{R}\|_F = 0$$

For "non-T-based" IntraOrthos, must have $\|I - \bar{Q}^T \bar{Q}\|_F \leq O(\varepsilon)$

- HouseQR, CGSI+, TSQR, …

- What about BMGS-SVL with IntraOrthos that don't produce T's?

- Implicitly, they produce $\bar{T} = I$

- In this case,

$$\|\Delta_{TS}\|_F = \|\bar{T}S - I\|_F = \|\mathrm{I} - \mathrm{triu}(\bar{Q}^T\bar{Q})\|_F \leq \|I - \bar{Q}^T\bar{Q}\|_F$$
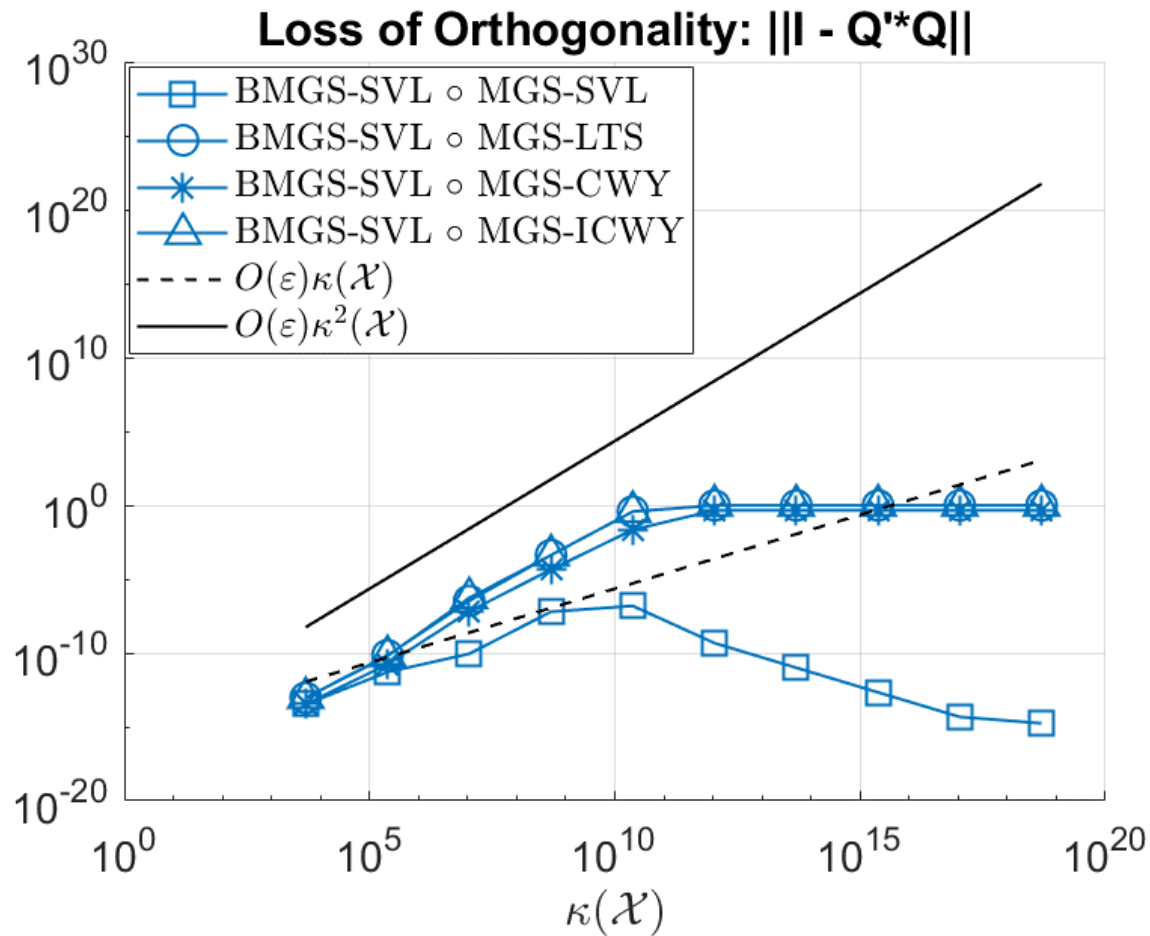
$$\left\|\Delta_{\bar{Q}\bar{R}}\right\|_F = \|\bar{Q}\bar{R} - X\|_F$$

$$\|\Gamma_{TR}\|_F = \|(I - \bar{T})\bar{R}\|_F = 0$$

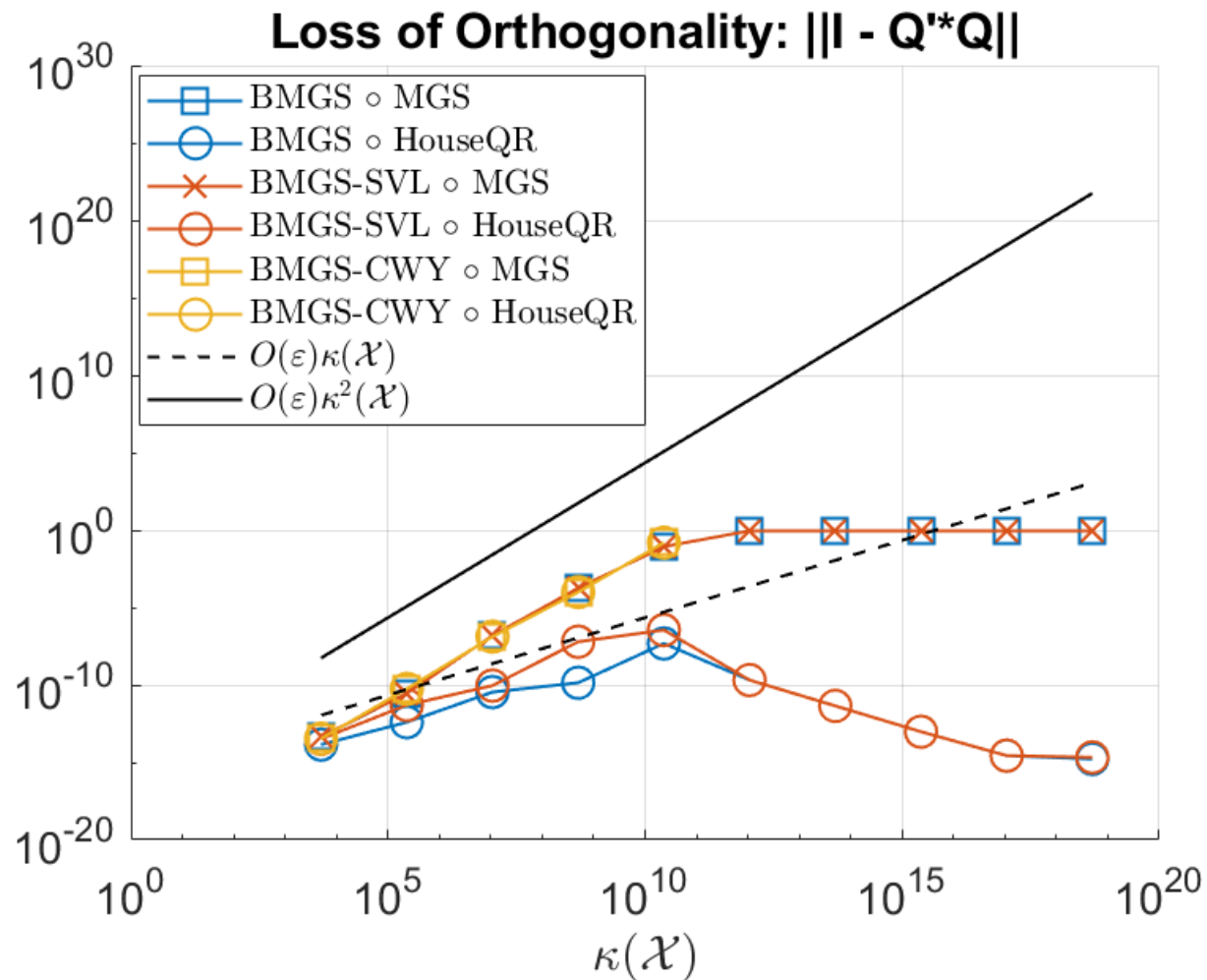For "non-T-based" IntraOrthos, must have $\|I - \bar{Q}^T\bar{Q}\|_F \leq O(\varepsilon)$

- HouseQR, CGSI+, TSQR, …

- What about BMGS with another T-variant IntraOrtho?

Läuchli matrix
$m = 1000, p = 100, s = 5$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BMGS-SVL ∘ MGS-SVL
- BMGS-SVL ∘ MGS-LTS
- BMGS-SVL ∘ MGS-CWY
- BMGS-SVL ∘ MGS-ICWY
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

```
LaeuchliBlockKappaPlot([1000 100 5],  logspace(-1, -16, 10), {'BMGS_SVL'}, {'MGS_SVL','MGS_LTS','MGS_CWY','MGS_ICWY'})
```

Läuchli matrix
$$m = 1000, p = 100, s = 5$$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BMGS ∘ MGS
- BMGS ∘ HouseQR
- BMGS-SVL ∘ MGS
- BMGS-SVL ∘ HouseQR
- BMGS-CWY ∘ MGS
- BMGS-CWY ∘ HouseQR
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$

```
LaeuchliBlockKappaPlot([1000 100 5], logspace(-1, -16, 10), {'BMGS','BMGS_SVL','BMGS_CWY'}, {'MGS','HouseQR'})
```
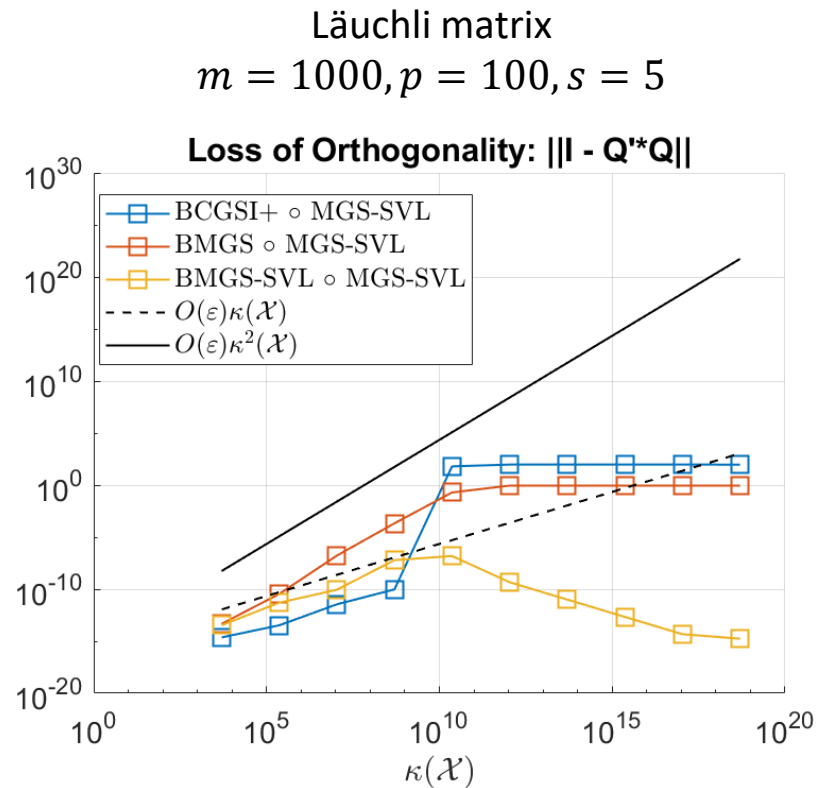
The "T fix"

- Both BCGSI+ and BMGS suffer total loss of orthogonality with MGS-SVL as IntraOrtho

Läuchli matrix
$$m = 1000, p = 100, s = 5$$

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- BMGS ∘ MGS-SVL
- BMGS-SVL ∘ MGS-SVL
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$

LaeuchliBlockKappaPlot([1000 100 5], logspace(-1, -16, 10), {'BCGS_IRO','BMGS','BMGS_SVL'}, {'MGS_SVL'})
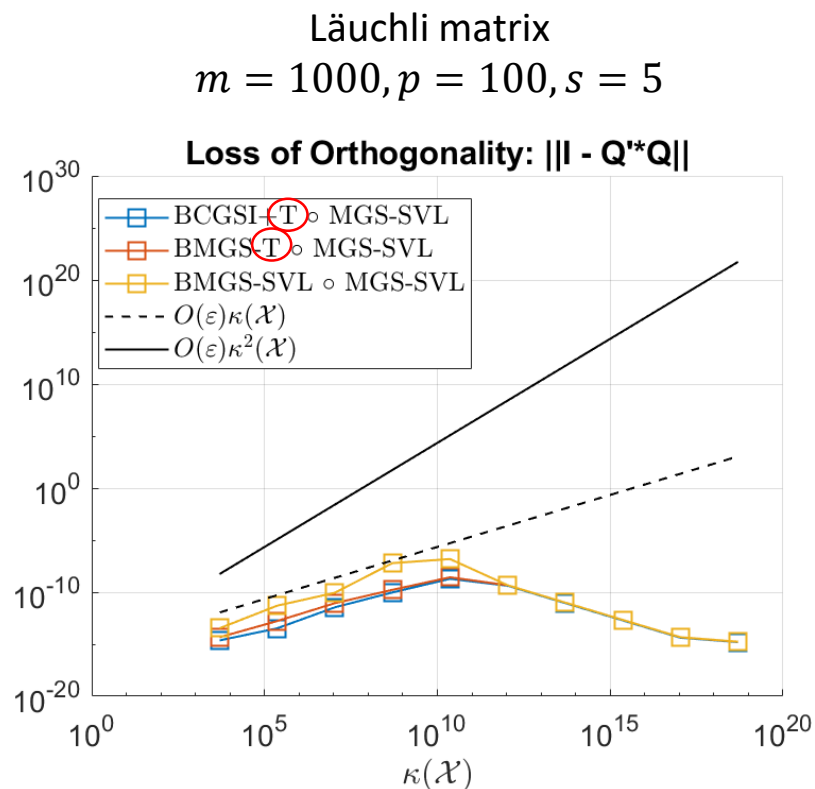
The "T fix"

- Both BCGSI+ and BMGS suffer total loss of orthogonality with MGS-SVL as IntraOrtho

- Fix:

  - Incorporate the T matrix output by MGS-SVL into the skeletons: Replace Q_k with $Q_k T_{k,k}$ everywhere

  - This leads to variants we call BCGSI+T and BMGS-T

Läuchli matrix
$$m = 1000, p = 100, s = 5$$

LaeuchliBlockKappaPlot([1000 100 5], logspace(-1, -16, 10), {'BCGS_IRO','BMGS','BMGS_SVL'}, {'MGS_SVL'})

The "T fix"

- Both BCGSI+ and BMGS suffer total loss of orthogonality with MGS-SVL as IntraOrtho

- Fix:

  - Incorporate the T matrix output by MGS-SVL into the skeletons: Replace Q_k with $Q_k T_{k,k}$ everywhere

  - This leads to variants we call BCGSI+T and BMGS-T

- BCGSI+T and BMGS-T perform similarly to BMGS-SVL

- Note: BMGS-SVL = BCGS + "T fix"

- Note: If these skeletons used with an IntraOrtho that doesn't produce a T, then $T = I$, so there is no difference

Läuchli matrix
$m = 1000, p = 100, s = 5$

Loss of Orthogonality: ||I - Q'*Q||

Legend:
- BCGSI+T ∘ MGS-SVL
- BMGS-T ∘ MGS-SVL
- BMGS-SVL ∘ MGS-SVL
- $O(\varepsilon)\kappa(\mathcal{X})$
- $O(\varepsilon)\kappa^2(\mathcal{X})$

x-axis: $\kappa(\mathcal{X})$

`LaeuchliBlockKappaPlot([1000 100 5],  logspace(-1, -16, 10), {'BCGS_IRO_T','BMGS_T','BMGS_SVL'}, {'MGS_SVL'})`

BMGS Variants

Algorithm	IntraOrtho reqs.	$\lVert I - \bar{Q}^T \bar{Q} \rVert$	Assumption on $\kappa(\mathcal{X})$	References
BMGS	$O(\varepsilon)$	$O(\varepsilon)\kappa(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	[Jalby and Philippe, 1991]
	$O(\varepsilon)\kappa(X)$	$O(\varepsilon)\kappa^2(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	[Jalby and Philippe, 1991]
BMGS-SVL	$O(\varepsilon)$ or MGS-SVL	$O(\varepsilon)\kappa(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	[Barlow, 2019]
BMGS-LTS	$O(\varepsilon)$ or MGS-LTS	$O(\varepsilon)\kappa(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	conjecture
BMGS-CWY	any	$O(\varepsilon)\kappa^2(\mathcal{X})$	$O(\varepsilon)\kappa^2(\mathcal{X}) < 1$	conjecture
BMGS-ICWY	any	$O(\varepsilon)\kappa^2(\mathcal{X})$	$O(\varepsilon)\kappa^2(\mathcal{X}) < 1$	conjecture
BMGS-T	$O(\varepsilon)$ or MGS-SVL	$O(\varepsilon)\kappa(\mathcal{X})$	$O(\varepsilon)\kappa(\mathcal{X}) < 1$	conjecture

Open Questions

Looking forward…

- Much work to do in proving stability, in particular for low-sync variants
  - What is the effect of normalization lag?
  - What skeletons work with what muscles?
- Randomized Gram-Schmidt variants [Balabanov, Grigori, 2020]
- Opportunities for mixed precision?
  - [Yamazaki, Tomov, Kurzak, Dongarra, Barlow, 2015]: mixed precision CholQR within BMGS and BCGS
  - [Yang, Fox, Sanders, 2019]: mixed precision HouseQR

- What are the necessary and sufficient conditions on degree of orthogonality in order to have backward stable block GMRES? Communication-avoiding GMRES?

Thank You!

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Survey paper: https://arxiv.org/pdf/2010.12058.pdf
BCGS-P variants: http://www.math.cas.cz/fichier/preprints/IM_20210124200723_43.pdf
BlockStab MATLAB package: https://github.com/katlund/BlockStab