The Numerical Stability of Block CGS Variants

Erin C. Carson, Kathryn Lund
Faculty of Mathematics and Physics, Charles University
Miro Rozložník
Institute of Mathematics, Czech Academy of Sciences

FACULTY
OF MATHEMATICS
AND PHYSICS
Charles University

May 18, 2021

SIAM LA 21

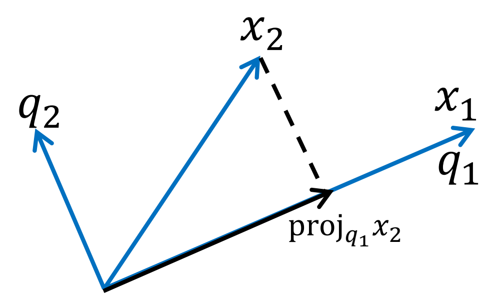
The Gram-Schmidt process

Given a set of linear independent vectors $x_1, \dots, x_n$, we want to compute a set of orthogonal vectors $q_1, \dots, q_n$ such that $span\{x_1, \dots, x_n\} = span\{q_1, \dots, q_n\}$

Gram-Schmidt process:

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

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 $q_1, \dots, q_k$.

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.

Finite Precision

- 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 having orthonormal columns?

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

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

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

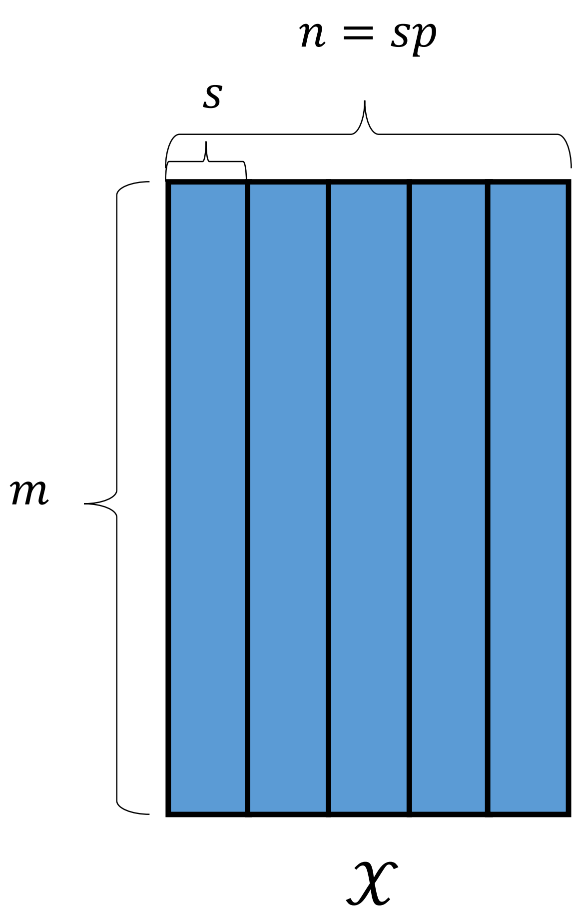
How close is $\bar{R}^T\bar{R}$ to X^TX?

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

Block Gram-Schmidt

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

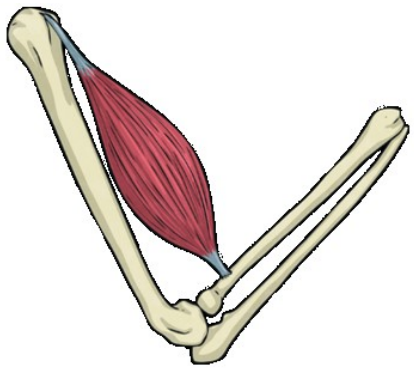
- Performance reasons (e.g., BLAS3)
- Block Krylov subspace methods
  - Better convergence
  - Simultaneously solve multiple RHSes
- s-step Krylov subspace methods



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 CGS (BCGS) for orthogonalizing between blocks, Householder QR for orthogonalizing within blocks:

$$\mathrm{BCGS} \circ \mathrm{HouseQR}(\mathcal{X})$$

Notation

- 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

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

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

Notation

- 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

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

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

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

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

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

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

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

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

$$\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)\kappa^2(X)$$

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

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

$$\|I - \bar{Q}^T\bar{Q}\| \leq O(\varepsilon)\kappa^2(X)$$

- [Smoktunowicz, Barlow, Langou, 2006]: The above only holds if we compute the diagonal entries of R using a Cholesky-like formula via the Pythagorean theorem (CGS-P)

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

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

$$\|I - \bar{Q}^T\bar{Q}\| \leq O(\varepsilon)\kappa^2(X)$$

- [Smoktunowicz, Barlow, Langou, 2006]: The above only holds if we compute the diagonal entries of R using a Cholesky-like formula via the Pythagorean theorem (CGS-P)

$$\begin{aligned} R_{1:k,k+1} &= Q_{1:k}^T x_{k+1} \\ w &= x_{k+1} - Q_{1:k}R_{1:k,k+1} \end{aligned}$$

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

CGS:

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

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

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

$$\|I - \bar{Q}^T \bar{Q}\| \leq O(\varepsilon)\kappa^2(X)$$

- [Smoktunowicz, Barlow, Langou, 2006]: The above only holds if we compute the diagonal entries of R using a Cholesky-like formula via the Pythagorean theorem (CGS-P)

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

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

CGS:

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

CGS-P:

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

Block CGS

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

$[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$

for $k = 1, \dots, p-1$ **do**

  $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$

  $\boldsymbol{W} = \boldsymbol{X}_{k+1} - \boldsymbol{\mathcal{Q}}_{1:k} \mathcal{R}_{1:k,k+1}$

  $[\boldsymbol{Q}_{k+1}, R_{k+1,k+1}] = \texttt{IntraOrtho}\,(\boldsymbol{W})$

end for

return $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \dots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

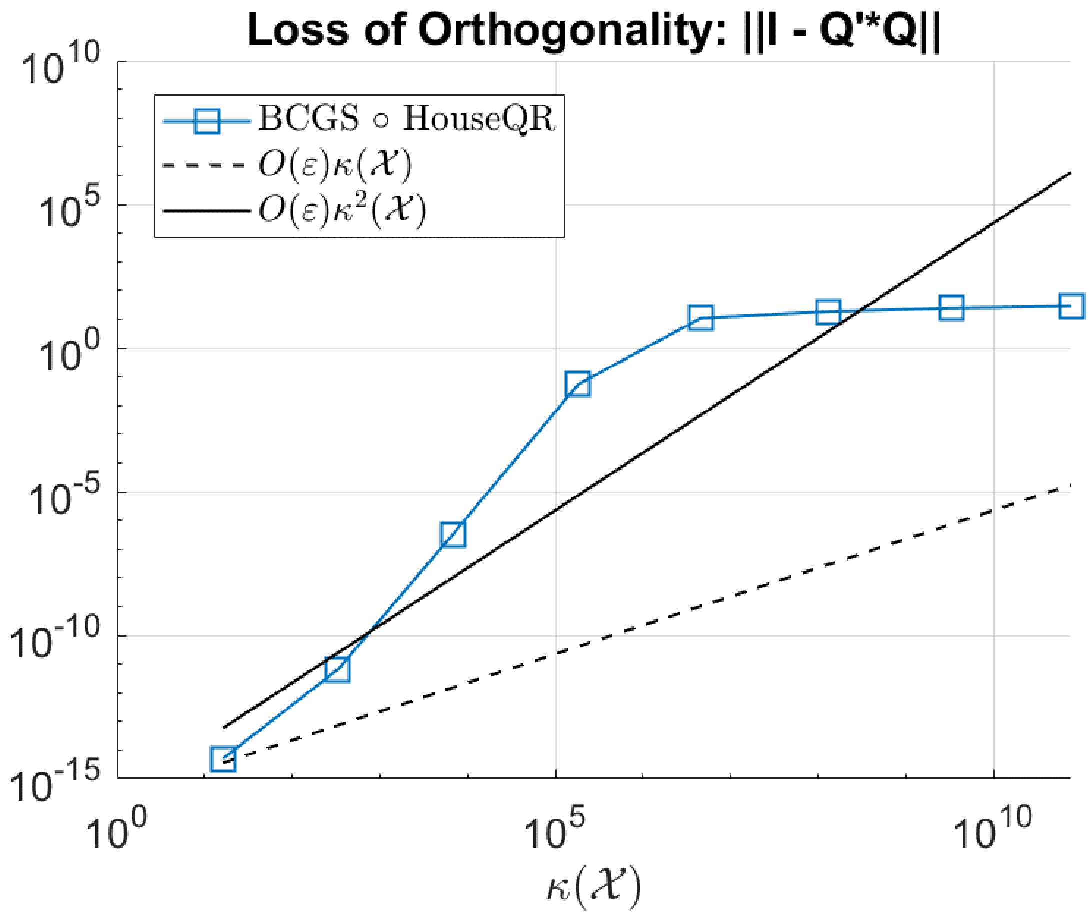
No existing proof of the loss of orthogonality in BCGS!

Conjecture: Even if our IntraOrtho has $O(\varepsilon)$ loss of orthogonality, BCGS is just as bad as CGS:

$$\|I - \bar{\mathcal{Q}}^T \bar{\mathcal{Q}}\| \le O(\varepsilon)\kappa^{n-1}(\mathcal{X})$$

"Glued" matrices from [Smoktunowicz, Barlow, Langou, 2006]

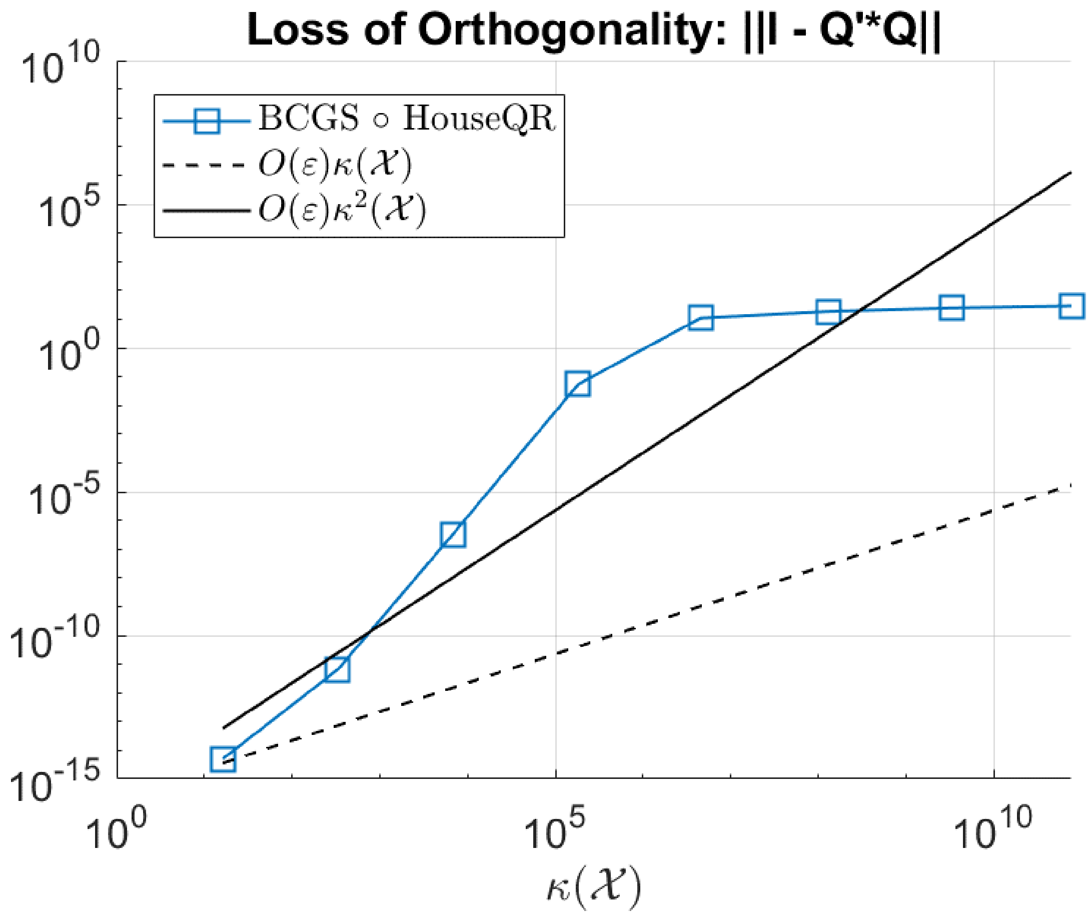
$m = 1000, p = 50, s = 4$



BlockStab MATLAB package: https://github.com/katlund/BlockStab

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

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



BCGS loss of orthogonality is ***not*** $O(\varepsilon)\kappa^2(\mathcal{X})$!

BlockStab MATLAB package: https://github.com/katlund/BlockStab

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

Block Pythagorean CGS

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

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

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

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

Block Pythagorean CGS

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

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

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

$[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$

for $k = 1, \ldots, p-1$ **do**

  $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$

end for

return $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

Block Pythagorean CGS

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

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

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

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

$[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$

for $k = 1, \ldots, p-1$ **do**

$\quad \mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$

end for

return $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

Block Pythagorean CGS

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

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

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

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}

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

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

Block Pythagorean CGS

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

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

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

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

[$\boldsymbol{Q}_1, R_{11}$] $= \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$

for $k = 1, \ldots, p-1$ **do**

  $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$

end for

return $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

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}

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

Block Pythagorean CGS

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

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

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

$[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$

for $k = 1, \ldots, p-1$ **do**

  $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$

end for

return $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

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

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}

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

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

Block Pythagorean CGS

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

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

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

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}

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

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

```
[Q_1, R_11] = IntraOrtho(X_1)
for k = 1, ..., p-1 do
    R_{1:k,k+1} = Q_{1:k}^T X_{k+1}

end for
return Q = [Q_1, ..., Q_p], R = (R_jk)
```

Block Pythagorean CGS

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

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

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

$[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$

for $k = 1, \ldots, p-1$ **do**

  $\mathcal{R}_{1:k,k+1} = \boldsymbol{\mathcal{Q}}_{1:k}^T \boldsymbol{X}_{k+1}$

end for

return $\boldsymbol{\mathcal{Q}} = [\boldsymbol{Q}_1, \ldots, \boldsymbol{Q}_p]$, $\mathcal{R} = (R_{jk})$

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

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}

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

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

Block Pythagorean CGS

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

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

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

1: $[Q_1, R_{11}] = \texttt{IntraOrtho}\,(X_1)$

2: **for** $k = 1, \ldots, p-1$ **do**

3: $\quad \mathcal{R}_{1:k,k+1} = \mathcal{Q}_{1:k}^T X_{k+1}$

6: **end for**

7: **return** $\mathcal{Q} = [Q_1, \ldots, Q_p]$, $\mathcal{R} = (R_{jk})$

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

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}

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

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

BCGS-PIP and BCGS-PIO

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

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

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

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

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

$[\boldsymbol{Q}_1, R_{11}] = \texttt{IntraOrtho}\,(\boldsymbol{X}_1)$
for $k = 1, \dots, p-1$ **do**
  $\mathcal{R}_{1:k,k+1} = \mathcal{Q}_{1:k}^T \boldsymbol{X}_{k+1}$
  $\left[\sim, \begin{bmatrix} T_{k+1} & \\ & P_{k+1} \end{bmatrix}\right] = \texttt{IntraOrtho}\left(\begin{bmatrix} \boldsymbol{X}_{k+1} & \\ & \mathcal{R}_{1:k,k+1} \end{bmatrix}\right)$
  $\boldsymbol{W}_{k+1} = \boldsymbol{X}_{k+1} - \mathcal{Q}_{1:k}\mathcal{R}_{1:k,k+1}$
  $\boldsymbol{Q}_{k+1} = \boldsymbol{W}_{k+1} R_{k+1,k+1}^{-1}$
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"

New Stability Results for BCGS-PIP/PIO

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

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

Suppose we execute BCGS-PIP ∘ IntraOrtho($\mathcal{X}$) or BCGS-PIO ∘ IntraOrtho($\mathcal{X}$).

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

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

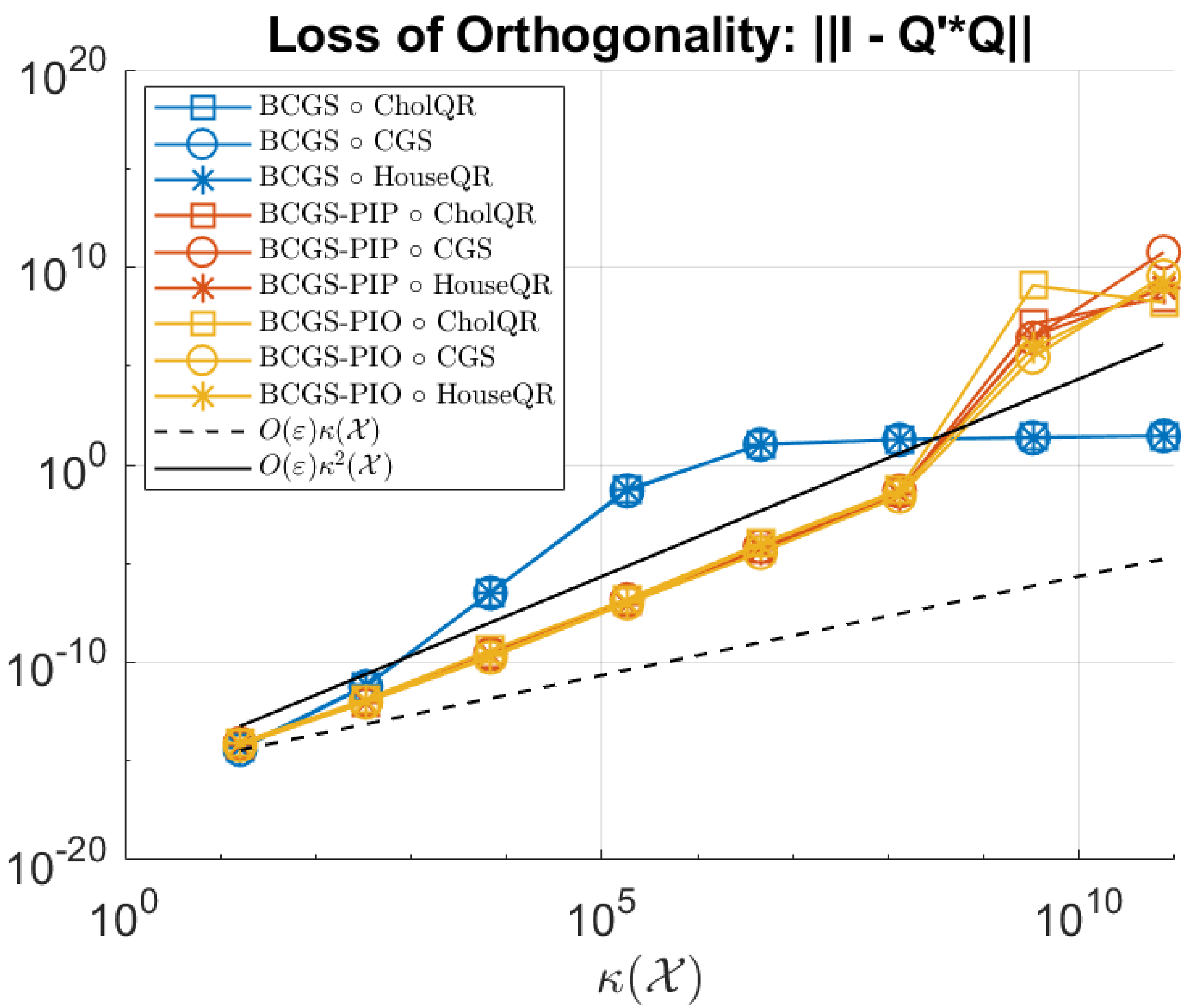
then the factors $\bar{\mathcal{Q}}$ and $\bar{\mathcal{R}}$ satisfy

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

[C., Lund, Rozložník, 2021]

“Glued” matrices from [Smoktunowicz, Barlow, Langou, 2006]

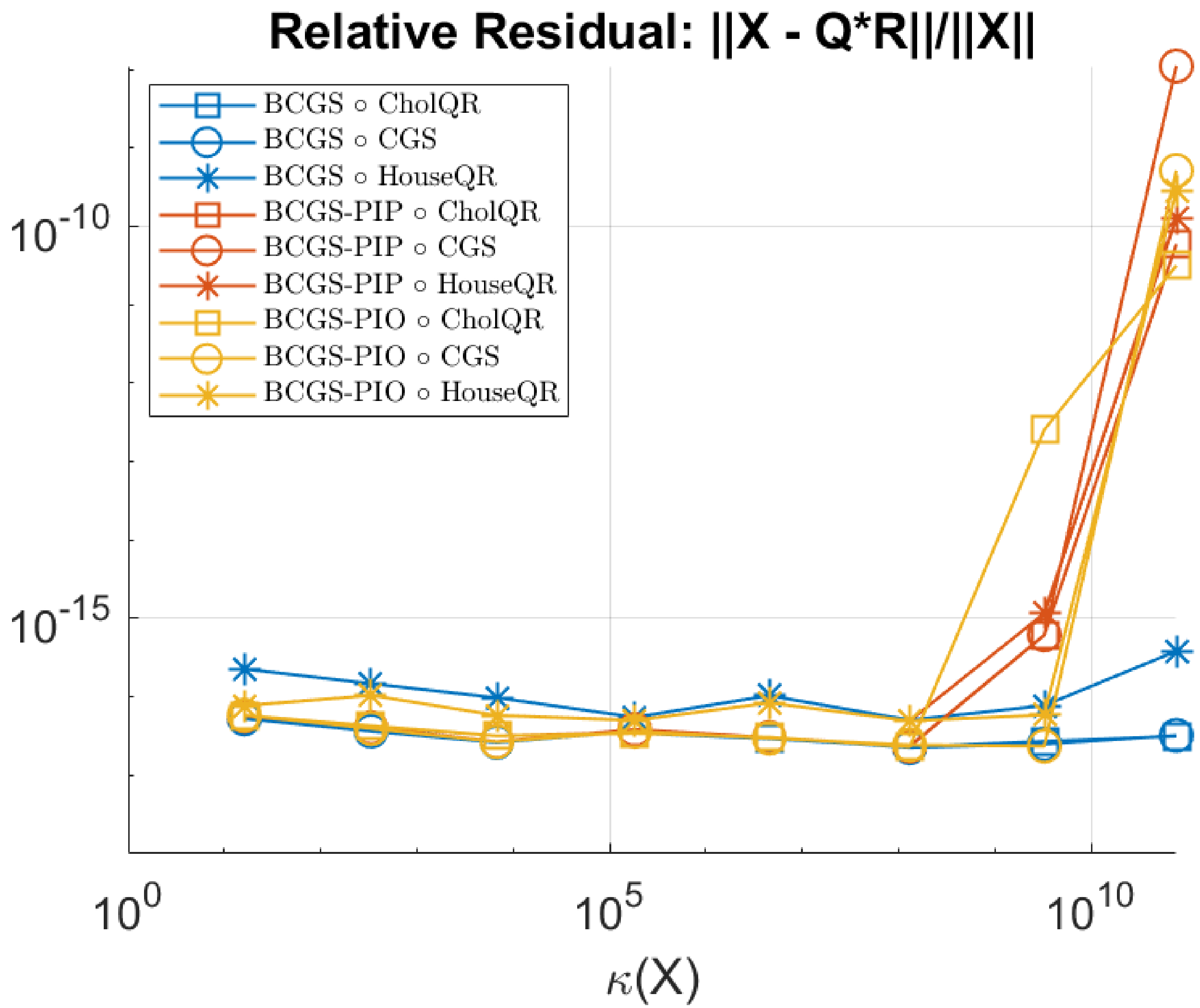
$m = 1000, p = 50, s = 4$




```
GluedBlockKappaPlot([1000 50 4], 1:8, {'BCGS', 'BCGS_PIP_FREE', 'BCGS_PIO_FREE'}, {'CHOLQR','CGS','HouseQR'})
```

“Glued” matrices from [Smoktunowicz, Barlow, Langou, 2006]

$m = 1000, p = 50, s = 4$




```
GluedBlockKappaPlot([1000 50 4], 1:8, {'BCGS', 'BCGS_PIP_FREE', 'BCGS_PIO_FREE'}, {'CHOLQR','CGS','HouseQR'})
```

Looking forward...

- Can we loosen the constraint on condition number (e.g., to $O(\varepsilon)\kappa(\mathcal{X}) < 1$)?
  - Need a better Cholesky:
  - [Yamazaki, Tomov, Kurzak, Dongarra, Barlow, 2015]: mixed precision CholeskyQR
  - [Fukaya, Kannan, Nakatsukasa, Yamamoto, Yanagisawa, 2020]: shifted-CholeskyQR3

- Stability for low-sync variants? [Świrydowicz, Langou, Ananthan, Yang, Thomas, 2021]
  - What is the effect of normalization lag?
  - What skeletons work with what muscles?

Thank You!

carson@karlin.mff.cuni.cz
www.karlin.mff.cuni.cz/~carson/

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