GRAM-SCHMIDT ORTHOGONALIZATION
WITH STANDARD AND NON-STANDARD INNER PRODUCT: ROUNDING ERROR ANALYSIS

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SIAM Conference on Applied Linear Algebra, Valencia, Spain, June 18-22, 2012

$$A = (a_1, \ldots, a_n) \in \mathcal{R}^{m,n}, \quad m \geq rank(A) = n$$

orthogonal basis Q of $span(A)$
$$Q = (q_1, \ldots, q_n) \in \mathcal{R}^{m,n}, Q^T Q = I$$

$A = QR$, R upper triangular ($A^T A = R^T R$)

finite precision arithmetic:
$$\bar{Q} = (\bar{q}_1, \ldots, \bar{q}_n), \ \bar{Q}^T\bar{Q} \neq I_n, \ \|I - \bar{Q}^T\bar{Q}\| \leq ?$$

- ▶ **classical** and **modified** Gram-Schmidt are mathematically equivalent, but they have **"different"** numerical properties

- ▶ **classical** Gram-Schmidt can be **"quite unstable",** can **"quickly" lose** all semblance of **orthogonality**

- ▶ Gram-Schmidt with **reorthogonalization**: **"two-steps are enough"** to preserve the orthogonality to working accuracy

- **modified** Gram-Schmidt:
  assuming $\mathcal{O}(u)\kappa(A) < 1$
  $\|I - \bar{Q}^T\bar{Q}\| \leq \frac{\mathcal{O}(u)\kappa(A)}{1-\mathcal{O}(u)\kappa(A)}$

  Björck, 1967, Björck, Paige, 1992

- **classical** Gram-Schmidt:
  assuming $c_1 u \kappa(A) < 1$
  $\|I - \bar{Q}^T\bar{Q}\| \leq \frac{\mathcal{O}(u)\kappa^2(A)}{1-\mathcal{O}(u)\kappa(A)}$

  Giraud, van den Eshof, Langou, R, 2005
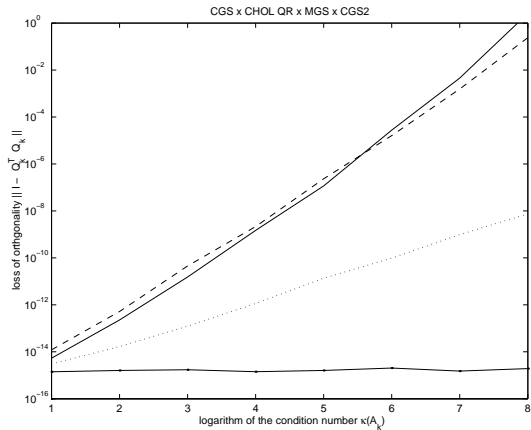 Barlow, Smoktunowicz, Langou, 2006

- classical or modified Gram-Schmidt with **reorthogonalization**:
  assuming $\mathcal{O}(u)\kappa(A) < 1$
  $\|I - \bar{Q}^T\bar{Q}\| \leq \mathcal{O}(u)$

  Giraud, van den Eshof, Langou, R, 2005
  Barlow, Smoktunowicz, 2011

CGS x CHOL QR x MGS x CGS2

loss of orthogonality $\| I - Q_k^T Q_k \|$

logarithm of the condition number $\kappa(A_k)$

Stewart, "Matrix algorithms" book, p. 284, 1998

$B \in \mathcal{R}^{m,m}$ symmetric positive definite, inner product $\langle \cdot, \cdot \rangle_B$
$A = [a_1, \ldots, a_n] \in \mathcal{R}^{m,n}$, $m \geq n = rank(A)$

B-orthogonal basis of the range of A:

$$Z = [z_1, \ldots, z_n] \in \mathcal{R}^{m,n}, Z^T B Z = I$$

$$A = ZU, U \in \mathcal{R}^{n,n} \text{ upper triangular}$$

$$A^T B A = U^T U$$

$$B^{1/2}A = (B^{1/2}Z)U, \ Z^TBZ = (B^{1/2}Z)^T(B^{1/2}Z) = I$$

$$\kappa(Z) \ll \kappa^{1/2}(B)$$

$$\kappa(U) = \kappa(B^{1/2}A) \le \kappa^{1/2}(B)\kappa(A)$$

finite precision arithmetic:
$$\bar{Z} = (\bar{z}_1, \ldots, \bar{z}_n), \ \bar{Z}^TB\bar{Z} \ne I, \ \|I - \bar{Z}^TB\bar{Z}\| \le ?$$
$$\bar{U}^T\bar{U} \approx A^TBA, \ \|A^TBA - \bar{U}^T\bar{U}\| \le ?$$
$$\bar{Z}\bar{U} \approx A, \ \|A - \bar{Z}\bar{U}\| \le ?$$

$$B = V\Lambda V^T, \ \Lambda^{1/2}V^T A = QU, \ Z = V\Lambda^{-1/2}Q$$

backward stable eigendecomposition + backward stable QR:

$$\|\bar{Z}^T B \bar{Z} - I\| \leq \mathcal{O}(u)\|B\|\|\bar{Z}\|^2$$

$$z_i^{(0)} = a_i, \quad z_i^{(j)} = z_i^{(j-1)} - \alpha_{ji}z_j, \quad j = 1,\ldots,i-1$$

$$z_i = z_i^{(i-1)}/\alpha_{ii}, \quad \alpha_{ii} = \|z_i^{(i-1)}\|_B$$

modified Gram-Schmidt $\equiv$ SAINV: $\alpha_{ji} = \langle z_i^{(j-1)}, z_j\rangle_B$
classical Gram-Schmidt: $\alpha_{ji} = \langle a_i, z_j\rangle_B$
AINV algorithm: $\alpha_{ji} = \langle z_i^{(j-1)}, a_j/\alpha_{jj}\rangle_B$

LOSS OF B-ORTHOGONALITY IN GRAM-SCHMIDT

modified Gram-Schmidt:

$$\mathcal{O}(u)\kappa(B)\kappa(B^{1/2}A) < 1$$

$$\|I - \bar{Z}^T B \bar{Z}\| \leq \frac{\mathcal{O}(u)\|B\|\|\bar{Z}\|^2\kappa(B^{1/2}A)}{1 - \mathcal{O}(u)\|B\|\|\bar{Z}\|^2\kappa(B^{1/2}A)}$$

classical Gram-Schmidt and AINV algorithm:

$$\mathcal{O}(u)\kappa(B)\kappa(B^{1/2}A)\kappa(A) < 1$$

$$\|I - \bar{Z}^T B \bar{Z}\| \leq \frac{\mathcal{O}(u)\|B\|^{1/2}\|\bar{Z}\|\kappa(B^{1/2}A)\kappa^{1/2}(B)\kappa(A)}{1 - \mathcal{O}(u)\|B\|^{1/2}\|\bar{Z}\|\kappa(B^{1/2}A)\kappa^{1/2}(B)\kappa(A)}$$

classical Gram-Schmidt with reorthogonalization:

$$\mathcal{O}(u)\kappa^{1/2}(B)\kappa(B^{1/2}A) < 1$$

$$\|I - \bar{Z}^T B \bar{Z}\| \leq \mathcal{O}(u)\|B\|\|\bar{Z}\|\|\bar{Z}^{(1)}\|$$

general positive definite B :

$$|\mathrm{fl}[\langle \bar{z}_i^{(j-1)}, \bar{z}_j \rangle_B] - \langle \bar{z}_i^{(j-1)}, \bar{z}_j \rangle_B| \leq \mathcal{O}(u)\|B\|\|\bar{z}_i^{(j-1)}\|\|\bar{z}_j\|$$
$$|1 - \|\bar{z}_j\|_B^2| \leq \mathcal{O}(u)\|B\|\|\bar{z}_j\|^2$$

diagonal positive (weight matrix) B :

$$|\mathrm{fl}[\langle \bar{z}_i^{(j-1)}, \bar{z}_j \rangle_B] - \langle \bar{z}_i^{(j-1)}, \bar{z}_j \rangle_B| \leq \mathcal{O}(u)\|\bar{z}_i^{(j-1)}\|_B\|\bar{z}_j\|_B$$
$$|1 - \|\bar{z}_j\|_B^2| \leq \mathcal{O}(u)$$

DIAGONAL CASE IS SIMILAR TO STANDARD CASE

modified Gram-Schmidt:

$$\mathcal{O}(u)\kappa(B^{1/2}A) < 1$$

$$\|I - \bar{Z}^T B \bar{Z}\| \leq \frac{\mathcal{O}(u)\kappa(B^{1/2}A)}{1 - \mathcal{O}(u)\kappa(B^{1/2}A)}$$

classical Gram-Schmidt and AINV algorithm

$$\mathcal{O}(u)\kappa^2(B^{1/2}A) < 1$$

$$\|I - \bar{Z}^T B \bar{Z}\| \leq \frac{\mathcal{O}(u)\kappa^2(B^{1/2}A)}{1 - \mathcal{O}(u)\kappa^2(B^{1/2}A)}$$

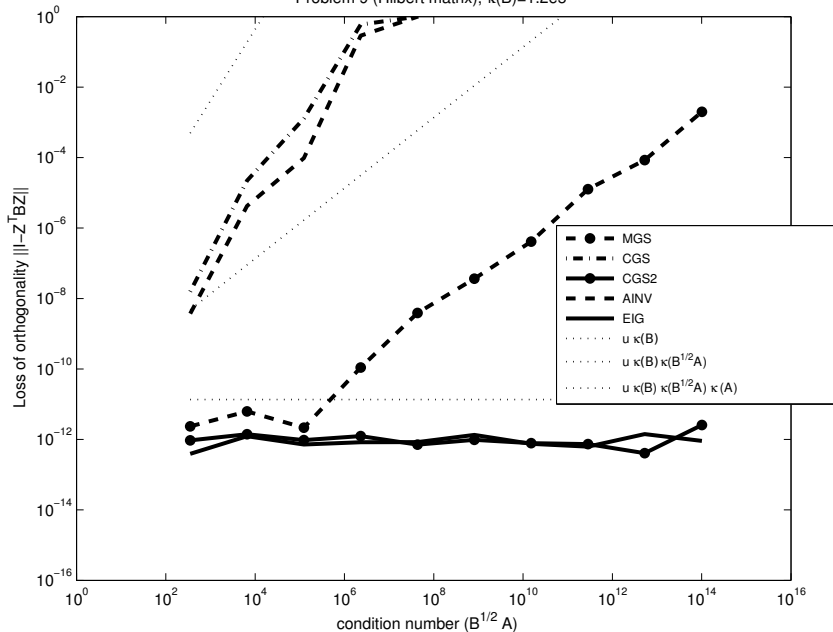classical Gram-Schmidt with reorthogonalization:

$$\mathcal{O}(u)\kappa(B^{1/2}A) < 1$$

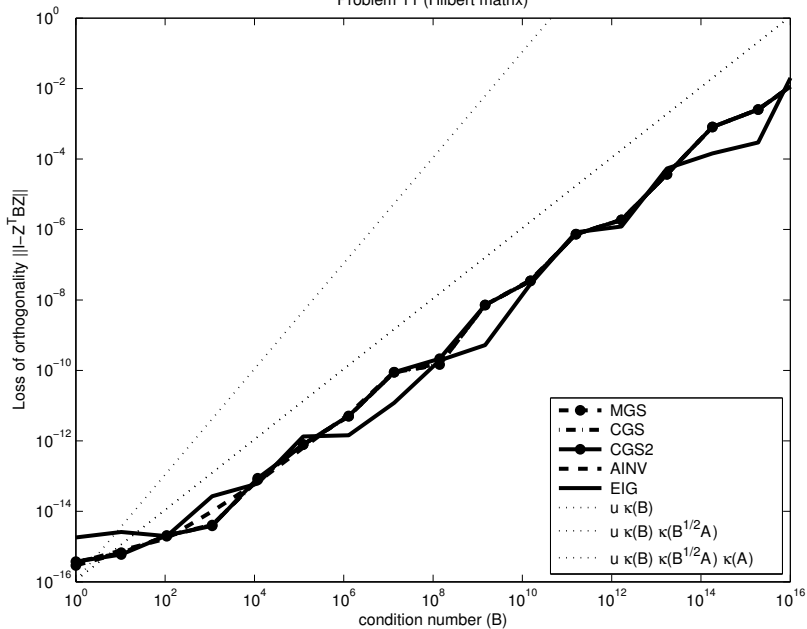$$\|I - \bar{Z}^T B \bar{Z}\| \leq \mathcal{O}(u)$$

Gulliksson, Wedin 1992, Gulliksson 1995

1. $\kappa^{1/2}(B) \ll \kappa(B^{1/2}A)$

2. $\kappa(B^{1/2}A) \leq \kappa^{1/2}(B)$
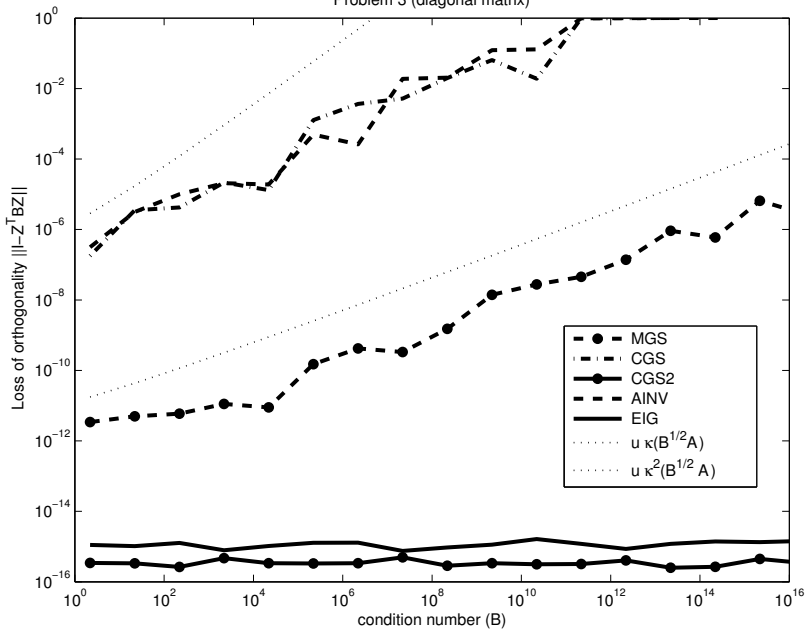
3. B positive diagonal

Problem 9 (Hilbert matrix), $\kappa(B)=1.2e5$

Problem 11 (Hilbert matrix)

Problem 3 (diagonal matrix)

ELEMENTARY SR FACTORIZATION

$$J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix} \in \mathcal{R}^{2m,2m} \text{ skew-symmetric and orthogonal}$$
$$A = [a_1, a_2] \in \mathcal{R}^{2m,2}, \text{ non-isotropic with } a_1^T J a_2 \neq 0$$

$$V = [v_1, v_2] \in \mathcal{R}^{2m,2}, \text{ symplectic } V^J V = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} V^T J V = I_2, v_1^T J v_2 = 1$$

$$A = VR, R = \begin{pmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{pmatrix} \in \mathcal{R}^{2,2} \text{ upper triangular with } r_{11} r_{22} = a_1^T J a_2$$

finite precision arithmetic:
$\bar{V} = (\bar{v}_1, \bar{v}_2),\ \bar{V}^J \bar{V} \neq I,\ |\bar{v}_1^T J \bar{v}_2 - 1| \leq ?$

loss of symplecticity:
assuming $|a_1^T J a_2| > \mathcal{O}(u) \|a_1\| \|a_2\|$

$$|\bar{v}_1^T J \bar{v}_2 - 1| \leq \frac{\mathcal{O}(u) \frac{\|a_1\| \|a_2\|}{|a_1^T J a_2|}}{1 - \mathcal{O}(u) \frac{\|a_1\| \|a_2\|}{|a_1^T J a_2|}}$$

Thank you for your attention!!!

Reference: J. Kopal, R, A. Smoktunowicz, and M. Tůma: Rounding error analysis of orthogonalization with a non-standard inner product, to appear in BIT.