GRAM-SCHMIDT PROCESS: FROM THE STANDARD TO THE NON-STANDARD INNER PRODUCT

Miro Rozložník

joint work with Jiří Kopal, Ahmed Salam, Alicja Smoktunowicz and Miroslav Tůma

Institute of Computer Science, Czech Academy of Sciences, Prague, Czech Republic

Structured Matrix Computations in Non-Euclidean Geometries: Algorithms and Applications, Luminy, France, October 8-12, 2012

STANDARD INNER PRODUCT: GRAM-SCHMIDT PROCESS AS QR ORTHOGONALIZATION

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

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

$A = QR$, 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

GRAM-SCHMIDT PROCESS VERSUS ROUNDING ERRORS

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

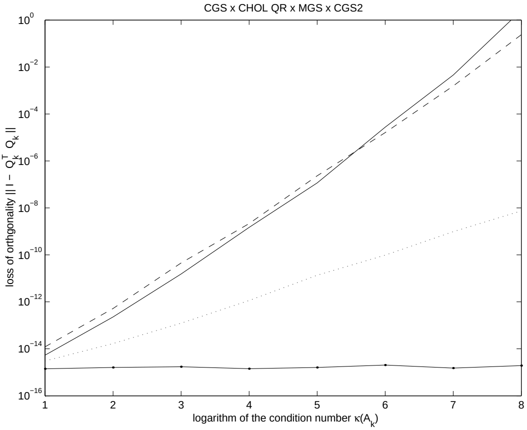
  Björck, 1967, Björck, Paige, 1992

- **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



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

ON THE WAY FROM THE STANDARD TO THE NONSTANDARD INNER PRODUCT

- Axel Ruhe. Numerical aspects of. Gram-Schmidt orthogonalization. of vectors. Lin. Alg. and its Appl.,. 52/53 (591-601), 1983.
- T. Ericsson, An analysis of orthogonalization in elliptic norms, to appear.
- M. Gulliksson: Backward error analysis for the constrained and weighted linear least squares problem when using the weighted QR factorization. SIAM J. Matrix Anal. Appl. 16(2), 675-687 (1995)
  M. Gulliksson: On the modified GramSchmidt algorithm for weighted and constrained linear least squares problems. BIT Numer. Math. 35(4), 453-468 (1995)
- S.J. Thomas, R.V.M. Zahar: Efficient orthogonalization in the M-norm. Congr. Numer. 80, 23-32 (1991) 36.
  S.J. Thomas, R.V.M. Zahar, : An analysis of orthogonalization in elliptic norms. Congr. Numer. 86, 193-222 (1992)

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

B-orthogonal basis of the range of A:

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

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

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

NON-STANDARD ORTHOGONALIZATION AND STANDARD QR

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

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

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

finite precision arithmetic:

$$\bar{Z} = (\bar{z}_1, \ldots, \bar{z}_n),\, \bar{Z}^TB\bar{Z} \neq I,\, \|I - \bar{Z}^TB\bar{Z}\| \leq ?$$

$$\bar{U}^T\bar{U} \approx A^TBA, \;\; \|A^TBA - \bar{U}^T\bar{U}\| \leq ?$$

$$\bar{Z}\bar{U} \approx A, \;\; \|A - \bar{Z}\bar{U}\| \leq ?$$

REFERENCE AND GRAM-SCHMIDT IMPLEMENTATIONS

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

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:

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

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

THE LOCAL ERRORS IN A NON-STANDARD INNER PRODUCTS

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:

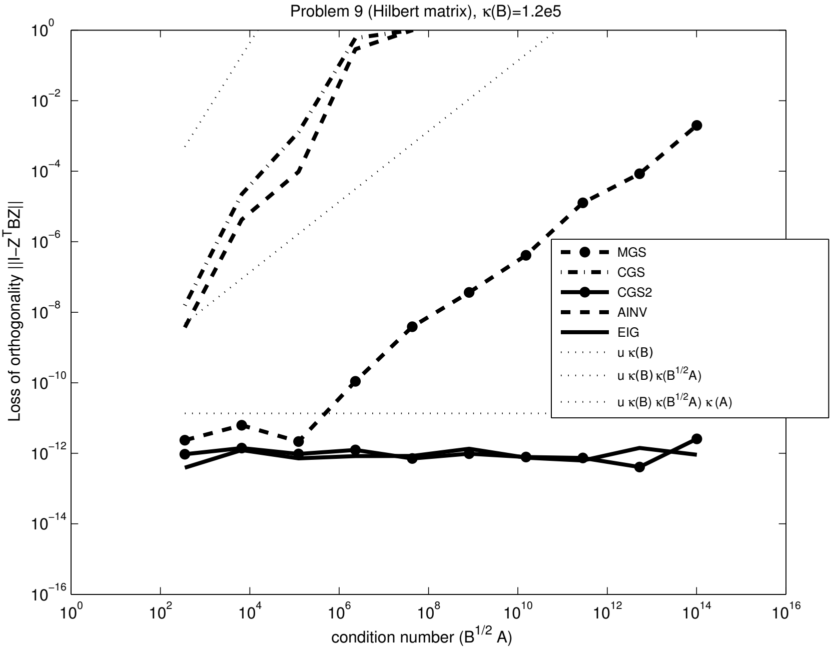
$$\mathcal{O}(u)\kappa(B^{1/2}A) < 1$$

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

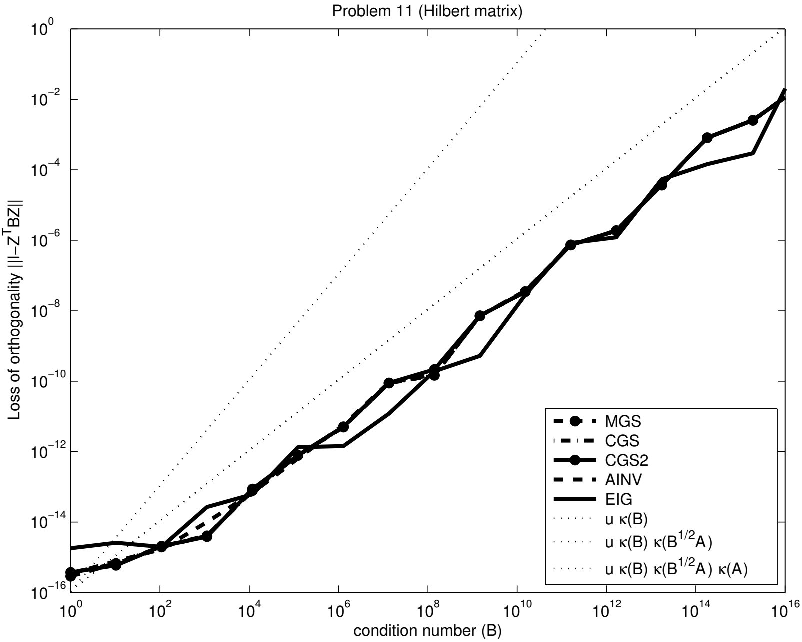
Gulliksson, Wedin 1992, Gulliksson 1995

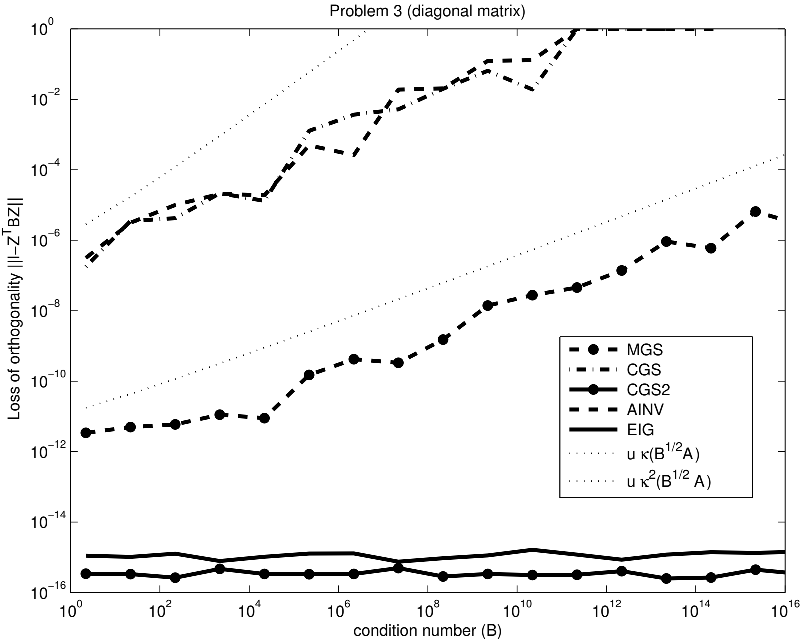
NUMERICAL EXPERIMENTS - EXTREMAL CASES

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), κ(B)=1.2e5
Loss of orthogonality ||I−Z^T BZ||
condition number (B^1/2 A)
MGS
CGS
CGS2
AINV
EIG
u κ(B)
u κ(B) κ(B^1/2 A)
u κ(B) κ(B^1/2 A) κ (A)


Problem 11 (Hilbert matrix)
Loss of orthogonality ||I−Z^T BZ||
condition number (B)
MGS
CGS
CGS2
AINV
EIG
u κ(B)
u κ(B) κ(B^1/2A)
u κ(B) κ(B^1/2A) κ(A)


Problem 3 (diagonal matrix)
Loss of orthogonality ||I−Z^T BZ||
condition number (B)
MGS
CGS
CGS2
AINV
EIG
u κ(B^1/2 A)
u κ^2(B^1/2 A)

ON THE WAY FROM THE INNER PRODUCT TO THE BILINEAR FORM

- Jose Román: Symmetric indefinite eigenvalue problems. The bilinear form $\langle x, y\rangle_B = y^T Bx$ can have $\langle x, x\rangle_B < 0$ and $\langle x, x\rangle_B = 0$ for some $x \neq 0$.
- Eigenvectors X can be chosen such that $X^T BX = \Omega$ where $\Omega = \mathrm{diag}(\pm 1)$ is a signature matrix. Isotropic vectors $x^T Bx = 0$.
- Structured eigenvalue problems. The SR factorization. The skew-symmetric bilinear form $\langle x, y\rangle_B = y^T Bx$, where $B^T = -B$. Each vector satisfies $x^T Bx = 0$.

ELEMENTARY SR FACTORIZATION

$$J = \begin{pmatrix} 0 & I_m \\ -I_m & 0 \end{pmatrix} \in \mathcal{R}^{2m,2m} \text{ skew-symmetric and orthogonal}$$

$$A = [a_1, a_2] \in \mathcal{R}^{2m,2}, \text{ non-isotropic with } a_1^T J a_2 \neq 0$$

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

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

GRAM-SCHMIDT WITH SKEW-SYMMETRIC BILINEAR FORM

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, BIT Numerical Mathematics, Online First.