Orthogonalization with a non-standard inner product and approximate inverse preconditioning

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Orthogonalization with a non-standard inner product

$A \in \mathcal{R}^{m,m}$ symmetric positive definite, inner product $\langle \cdot, \cdot \rangle_A$
$Z^{(0)} = [z_1^{(0)}, \ldots, z_n^{(0)}] \in \mathcal{R}^{m,n}$, $m \geq n = rank(Z^{(0)})$

A-orthogonal basis of $span(Z^{(0)})$:

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

$Z^{(0)} = ZU$, $U \in \mathcal{R}^{n,n}$ upper triangular

$$(Z^{(0)})^T A Z^{(0)} = U^T U$$

Non-standard orthogonalization and standard QR factorization

$$A^{1/2}Z^{(0)} = (A^{1/2}Z)U, \;\; Z^TAZ = (A^{1/2}Z)^T(A^{1/2}Z) = I$$

$$\kappa(Z) \leq \kappa^{1/2}(A)$$

$$\kappa(U) = \kappa(A^{1/2}Z^{(0)}) \leq \kappa^{1/2}(A)\kappa(Z^{(0)})$$

$Z^{(0)} = [e_1, \ldots, e_n]$: $Z = \begin{bmatrix} U^{-1} \\ 0 \end{bmatrix} \in \mathcal{R}^{m,n}$ upper triangular

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

Inverse factorization and approximate inverse preconditioning

$$ZZ^T = Z^{(0)}U^{-1}U^{-T}(Z^{(0)})^T = Z^{(0)}[(Z^{(0)})^T A Z^{(0)}]^{-1}(Z^{(0)})^T$$

AZZ^T : orthogonal projector onto $R(AZ^{(0)})$ and orthogonal to $R(Z^{(0)})$

$ZZ^T A$: orthogonal projector onto $R(Z^{(0)})$ and orthogonal to $R(AZ^{(0)})$

$Z^{(0)}$ square and nonsingular: inverse factorization $ZZ^T = A^{-1}$

$Ax = b$, approximate inverse $\bar{Z}\bar{Z}^T \approx A^{-1}$

$$\downarrow$$

$$\bar{Z}^T A \bar{Z} y = \bar{Z}^T b \ , \ \ x = \bar{Z} y, \ \ \|\bar{Z}^T A \bar{Z} - I\| \leq ?$$

$$\bar{U}^T \bar{U} \approx (Z^{(0)})^T A Z^{(0)}, \ \ \|(Z^{(0)})^T A Z^{(0)} - \bar{U}^T \bar{U}\| \leq ?$$

$$\bar{Z}\bar{U} \approx Z^{(0)}, \ \ \|Z^{(0)} - \bar{Z}\bar{U}\| \leq ?$$

Reference approach: Eigenvalue (EIG) based implementation

$$A = V\Lambda V^T, \;\; \Lambda^{1/2} V^T Z^{(0)} = QU, \;\; Z = V\Lambda^{-1/2} Q \text{ (or } Z = Z^{(0)} U^{-1}\text{)}$$

backward stable eigendecomposition + backward stable QR:

$$\|\bar{Z}^T A \bar{Z} - I\| \leq \mathcal{O}(u)\|A\|\|\bar{Z}\|^2$$
$$\|Z^{(0)} - \bar{Z}\bar{U}\| \leq \mathcal{O}(u)\|\bar{Z}\|\|\bar{U}\|$$
$$\|(Z^{(0)})^T A Z^{(0)} - \bar{U}^T \bar{U}\| \leq \mathcal{O}(u)\|A\|^{1/2}\|Z^{(0)}\|\|A^{1/2}Z^{(0)}\|$$

Practical algorithms: classical Gram-Schmidt (CGS) algorithm [Schmidt 1907, 1908], modified Gram-Schmidt (MGS) algorithm [Laplace 1816, Cauchy 1837], Gram-Schmidt with reorthogonalization [Kahan, Parlett, Kaufmann et al...]
Theory for standard inner product $A = I$: [MGS: Björck 1967, Björck and Paige 1992, CGS: Giraud, Langou, R, van den Eshof 2005, Barlow, Langou, Smoktunowicz 2006, CGS2: Giraud, Langou, R, van den Eshof 2005]

Gram-Schmidt orthogonalization

$$z_i^{(j)} = z_i^{(j-1)} - \alpha_{ji} z_j, \quad j = 1, \ldots, i-1$$
$$z_i = z_i^{(i-1)} / \alpha_{ii}, \quad \alpha_{ii} = \|z_i^{(i-1)}\|_A$$

modified Gram-Schmidt (MGS) algorithm $\equiv$ SAINV algorithm: $\alpha_{ji} = \langle z_i^{(j-1)}, z_j \rangle_A$
classical Gram-Schmidt (CGS) algorithm: $\alpha_{ji} = \langle z_i^{(0)}, z_j \rangle_A$
AINV algorithm: oblique projections $\alpha_{ji} = \langle z_i^{(j-1)}, z_j^{(0)} / \alpha_{jj} \rangle_A$

Approximate inverse preconditioning: from CGS in AINV to MGS in SAINV; various computation of diagonal entries [Benzi, Meyer, Tůma 1996; Benzi, Cullum, Tůma 2000; Benzi, Tůma 2003; Kharchenko, Kolotilina, Nikishin, Yeremin 2001]

Local errors in the (modified) Gram-Schmidt process

$$z_i^{(j)} = z_i^{(j-1)} - \alpha_{ji}\bar{z}_j$$

$$\alpha_{ji} = \langle z_i^{(j-1)}, \bar{z}_j \rangle_A$$

$$\langle z_i^{(j)}, \bar{z}_j \rangle_A = (1 - \|\bar{z}_j\|_A^2)\langle z_i^{(j-1)}, \bar{z}_j \rangle_A$$

$$z_i^{(j)} = z_i^{(j-1)} - \bar{\alpha}_{ji} z_j$$

$$\bar{\alpha}_{ji} = \mathrm{fl}[\langle z_i^{(j-1)}, z_j \rangle_A]$$

$$\langle z_i^{(j)}, z_j \rangle_A = \left(\mathrm{fl}[\langle z_i^{(j-1)}, z_j \rangle_A] - \langle z_i^{(j-1)}, z_j \rangle_A\right) \|z_j\|_A^2$$

Loss of orthogonality in the Gram-Schmidt algorithms

modified Gram-Schmidt algorithm:

$$\mathcal{O}(u)\kappa(A)\kappa(A^{1/2}Z^{(0)}) < 1$$

$$\|I - \bar{Z}^T A \bar{Z}\| \leq \frac{\mathcal{O}(u)\|A\|^{1/2}\|\bar{Z}\| \max_{i,j} \frac{\|A\|^{1/2}\|\bar{z}_i^{(j)}\|}{\|z_i^{(0)}\|_A} \kappa(A^{1/2}Z^{(0)})}{1 - \mathcal{O}(u)\|A\|^{1/2}\|\bar{Z}\| \max_{i,j} \frac{\|A\|^{1/2}\|\bar{z}_i^{(j)}\|}{\|z_i^{(0)}\|_A} \kappa(A^{1/2}Z^{(0)})}$$

classical Gram-Schmidt and AINV algorithm:

$$\mathcal{O}(u)\kappa(A)\kappa(A^{1/2}Z^{(0)})\kappa(Z^{(0)}) < 1$$

$$\|I - \bar{Z}^T A \bar{Z}\| \leq \frac{\mathcal{O}(u)\|A\|^{1/2}\|\bar{Z}\|\kappa(A^{1/2}Z^{(0)})\kappa^{1/2}(A)\kappa(Z^{(0)})}{1 - \mathcal{O}(u)\|A\|^{1/2}\|\bar{Z}\|\kappa(A^{1/2}Z^{(0)})\kappa^{1/2}(A)\kappa(Z^{(0)})}$$

Classical Gram-Schmidt (CGS2) with reorthogonalization

$$z_i^{(1)} = z_i^{(0)} - \sum_{j=1}^{i-1} \alpha_{ji}^{(1)} z_j, \quad \alpha_{ji}^{(1)} = \langle z_i^{(0)}, z_j \rangle_A$$

$$z_i^{(2)} = z_i^{(1)} - \sum_{j=1}^{i-1} \alpha_{ji}^{(2)} z_j, \quad \alpha_{ji}^{(2)} = \langle z_i^{(1)}, z_j \rangle_A$$

$$z_i = z_i^{(2)} / \alpha_{ii}, \quad \alpha_{ii} = \| z_i^{(2)} \|_A$$

$$\mathcal{O}(u) \kappa^{1/2}(A) \kappa(A^{1/2} Z^{(0)}) < 1$$

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

Twice-is-enough algorithm of Kahan-Parlett, iterated Gram-Schmidt process [Rice 1966, CGS2: Abdelmalek 1971, Daniel,Gragg, Kaufmann, Stewart 1976; Hoffman 1989; Giraud, Langou, R, van den Eshof 2005]

Local errors in the computation of inner products and normalization

general positive definite A :

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

diagonal (weight matrix) A :

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

A diagonal similar to orthogonalization with the standard inner product

MGS algorithm:

$$\mathcal{O}(u)\kappa(A^{1/2}Z^{(0)}) < 1$$

$$\|I - \bar{Z}^T A \bar{Z}\| \leq \frac{\mathcal{O}(u)\kappa(A^{1/2}Z^{(0)})}{1 - \mathcal{O}(u)\kappa(A^{1/2}Z^{(0)})}$$

CGS and AINV algorithms:

$$\mathcal{O}(u)\kappa^2(A^{1/2}Z^{(0)}) < 1$$

$$\|I - \bar{Z}^T A \bar{Z}\| \leq \frac{\mathcal{O}(u)\kappa^2(A^{1/2}Z^{(0)})}{1 - \mathcal{O}(u)\kappa^2(A^{1/2}Z^{(0)})}$$

CGS with reorthogonalization:

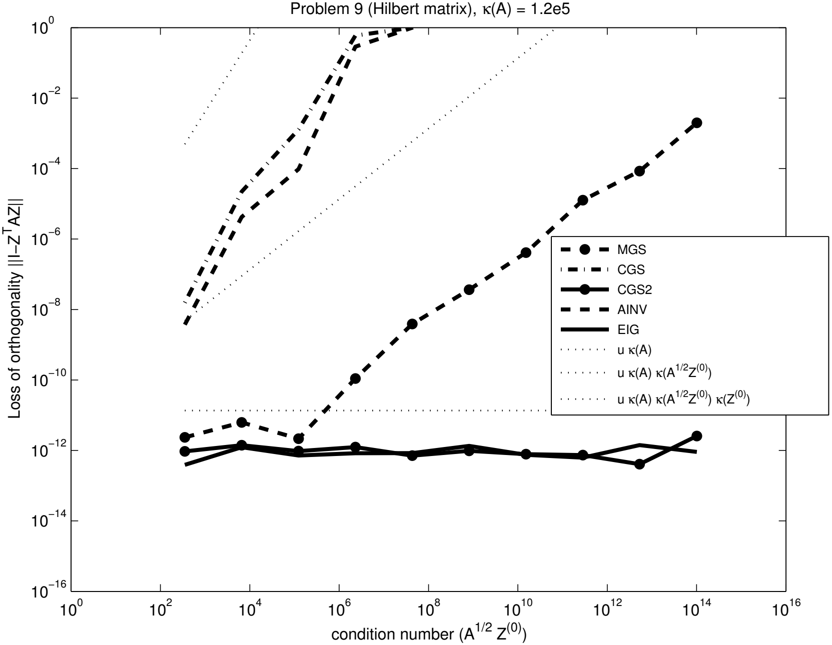
$$\mathcal{O}(u)\kappa(A^{1/2}Z^{(0)}) < 1$$

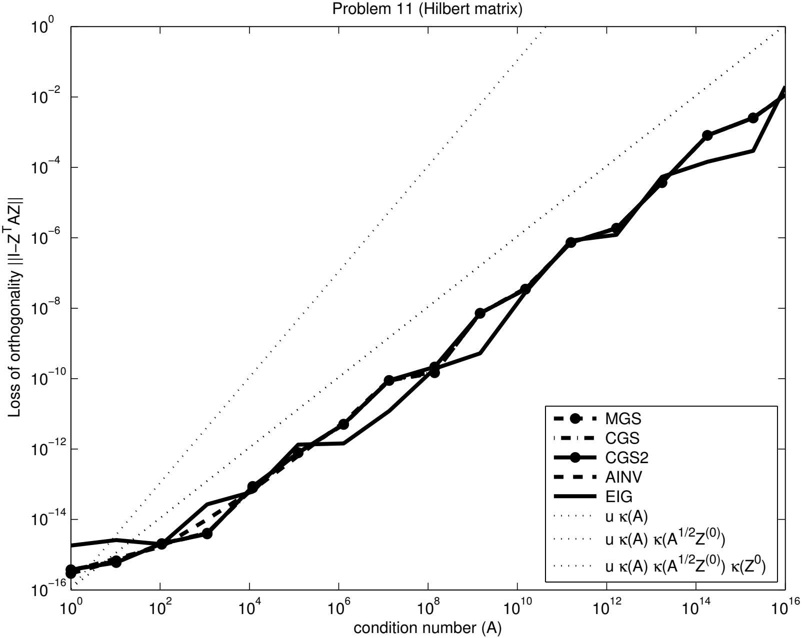
$$\|I - \bar{Z}^T A \bar{Z}\| \leq \mathcal{O}(u)$$

Weighted least squares problem; MGS: [Gulliksson, Wedin 1992, Gulliksson 1995]

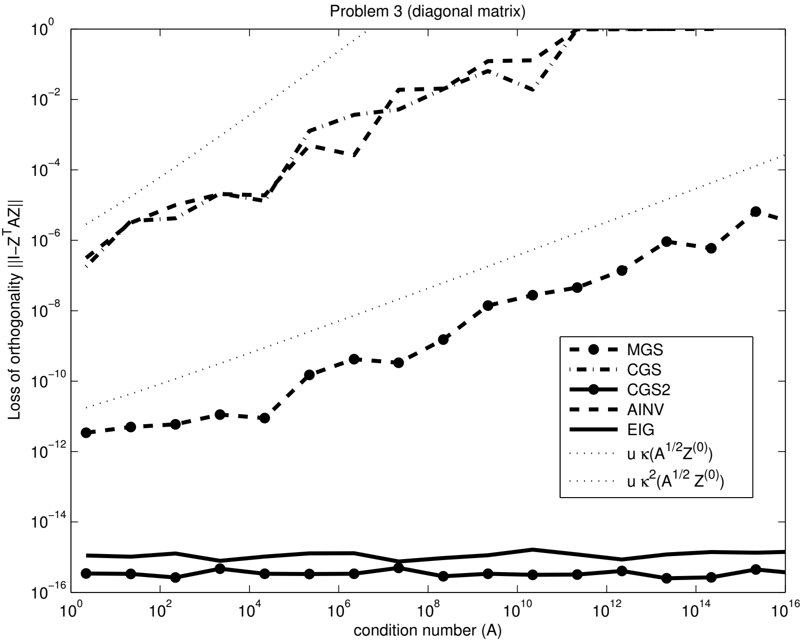
Numerical experiments - extremal cases

1. $\kappa^{1/2}(A) \ll \kappa(A^{1/2}Z^{(0)})$
2. $\kappa(A^{1/2}Z^{(0)}) \ll \kappa^{1/2}(A)$
3. A positive diagonal


Problem 9 (Hilbert matrix), κ(A) = 1.2e5
Loss of orthogonality ||I−Z^T AZ||
condition number (A^{1/2} Z^{(0)})
MGS
CGS
CGS2
AINV
EIG
u κ(A)
u κ(A) κ(A^{1/2}Z^{(0)})
u κ(A) κ(A^{1/2}Z^{(0)}) κ(Z^{(0)})



Problem 11 (Hilbert matrix)
Loss of orthogonality ||I−Z^T AZ||
condition number (A)
MGS
CGS
CGS2
AINV
EIG
u κ(A)
u κ(A) κ(A^{1/2}Z^{(0)})
u κ(A) κ(A^{1/2}Z^{(0)}) κ(Z^0)


Problem 3 (diagonal matrix)
Loss of orthogonality ||I−Z^T AZ||
condition number (A)
MGS
CGS
CGS2
AINV
EIG
u κ(A^{1/2}Z^{(0)})
u κ^2(A^{1/2} Z^{(0)})

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, submitted 2010.