

APPROXIMATE INVERSE PRECONDITIONING AND GRAM-SCHMIDT ORTHOGONALIZATION

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Orthogonalization with a non-standard inner product

$A \in \mathcal{R}^{m,m}$ symmetric positive definite, inner product $\langle \cdot, \cdot \rangle_A$

$Z^{(0)} = [z_1^{(0)}, \dots, z_n^{(0)}] \in \mathcal{R}^{m,n}$, $m \geq n = \text{rank}(Z^{(0)})$

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

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

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

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

Non-standard orthogonalization and standard QR factorization

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

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

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

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

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

Inverse factorization and approximate inverse preconditioning

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

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

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

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

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

$$\bar{Z}^TA\bar{Z}y = \bar{Z}^Tb, \quad x = \bar{Z}y, \quad \|\bar{Z}^TA\bar{Z} - I\| \leq ?$$

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

Reference approach: Eigenvalue (EIG) based implementation

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

backward stable eigendecomposition + backward stable QR:

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

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

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

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, Tuma 1996; Benzi, Cullum, Tuma 2000; Benzi, Tuma 2003; Kharchenko, Kolotilina, Nikishin, Yeremin 2001]

Local errors in the (modified) Gram-Schmidt process

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

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

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

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

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

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

Loss of orthogonality in the Gram-Schmidt algorithms

modified Gram-Schmidt algorithm:

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

classical Gram-Schmidt and AINV algorithm:

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

Classical Gram-Schmidt (CGS2) with reorthogonalization

$$\begin{aligned}z_i^{(1)} &= z_i^{(0)} - \sum_{j=1}^{i-1} \alpha_{ji}^{(1)} z_j, & \alpha_{ji}^{(1)} &= \langle z_i^{(0)}, z_j \rangle_A \\z_i^{(2)} &= z_i^{(1)} - \sum_{j=1}^{i-1} \alpha_{ji}^{(2)} z_j, & \alpha_{ji}^{(2)} &= \langle z_i^{(1)}, z_j \rangle_A \\z_i &= z_i^{(2)} / \alpha_{ii}, & \alpha_{ii} &= \|z_i^{(2)}\|_A\end{aligned}$$

$$\begin{aligned}\mathcal{O}(u) \kappa^{1/2}(A) \kappa(A^{1/2} Z^{(0)}) &< 1 \\ \|I - \bar{Z}^T A \bar{Z}\| &\leq \mathcal{O}(u) \|A\| \|\bar{Z}\| \|\bar{Z}^{(1)}\|\end{aligned}$$

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]

general positive definite A :

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

diagonal (weight matrix) A :

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

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:

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

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

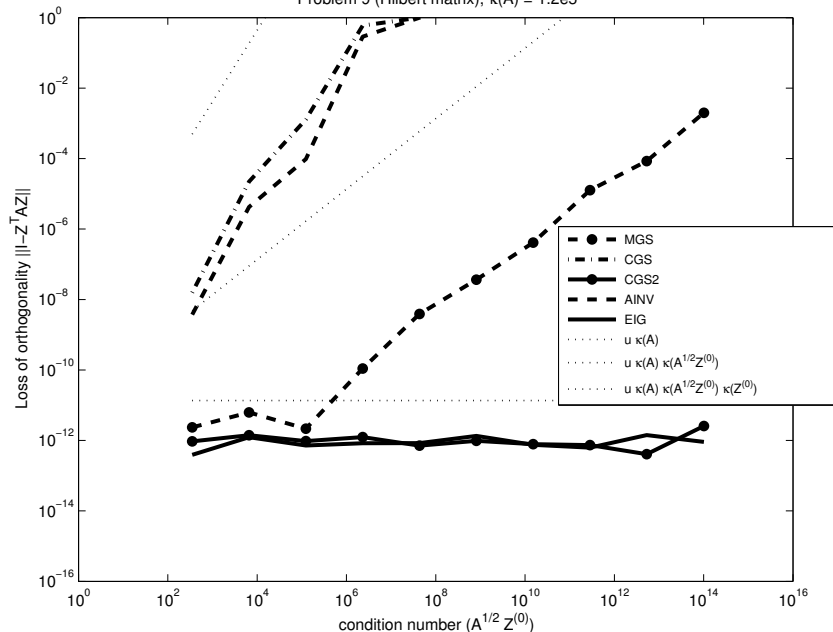
Weighted least squares problem; MGS: [Gulliksson, Wedin 1992, Gulliksson 1995]

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

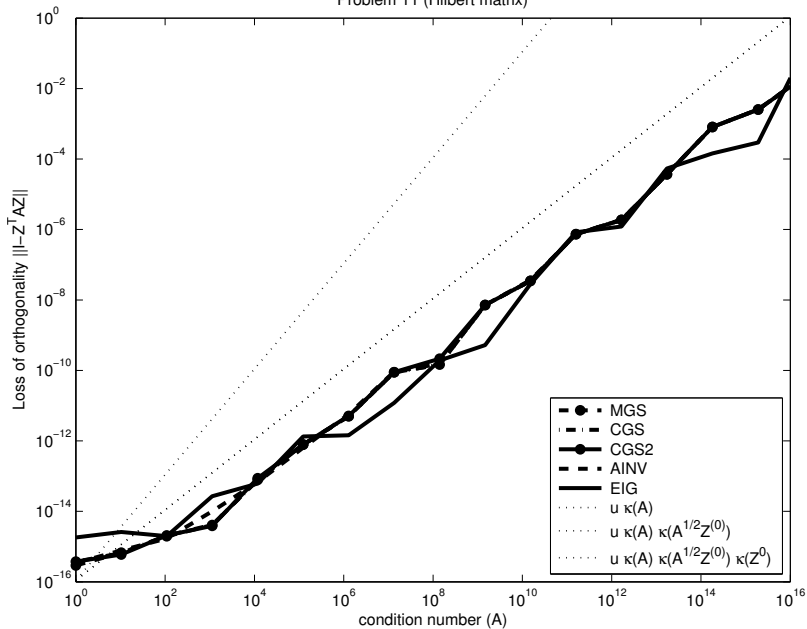
2. $\kappa(A^{1/2}Z^{(0)}) \ll \kappa^{1/2}(A)$

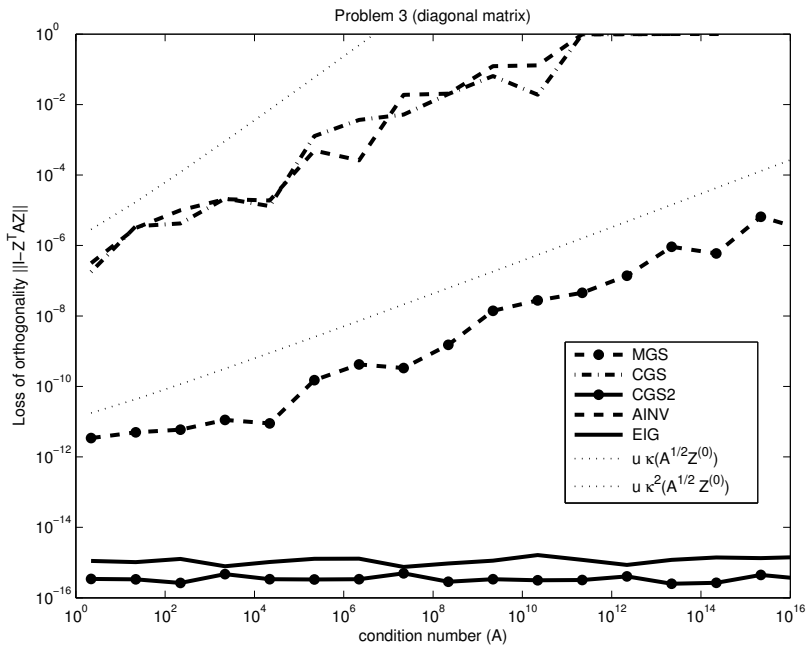
3. A positive diagonal

Problem 9 (Hilbert matrix), $\kappa(A) = 1.2\text{e}5$



Problem 11 (Hilbert matrix)





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.