ORTHOGONALIZATION WITH A NON-STANDARD INNER PRODUCT WITH THE APPLICATION TO PRECONDITIONING

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Orthogonalization with a non-standard inner product

A symmetric positive definite $m \times m$ matrix
$Z^{(0)} = [z_1^{(0)}, \ldots, z_n^{(0)}]$ full column rank $m \times n$ matrix
A-orthogonal basis of $span(Z^{(0)})$: $Z = [z_1, \ldots, z_n]$ - $m \times n$ matrix having orthogonal columns with respect to the inner product $\langle \cdot, \cdot \rangle_A$
U upper triangular $n \times n$ matrix

$$Z^{(0)} = ZU, \quad Z^T A Z = I$$

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

Condition number of orthogonal and triangular factor

$Z^T A Z = (A^{1/2}Z)^T(A^{1/2}Z) = I \Longrightarrow$
$A^{1/2}Z$ is orthogonal with respect to the standard inner product
$A^{1/2}Z^{(0)} = (A^{1/2}Z)U$ is a standard QR factorization

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

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

particular case $Z^{(0)} = I$: $Z = U^{-1}$ upper triangular $m \times n$ matrix

$$\kappa(U) = \kappa(Z)$$

Approximation properties of orthogonal factor

$$Z^T A Z = I$$

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

important case $Z^{(0)}$ square and nonsingular: inverse factorization

$$ZZ^T = A^{-1}$$

Important application: approximate inverse preconditioning

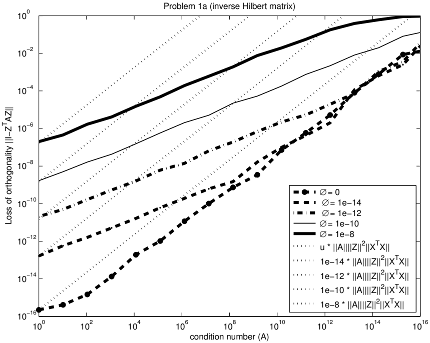
$\bar{Z}$ gives the approximate inverse $\bar{Z}\bar{Z}^T \approx A^{-1}$

$$Ax = b$$

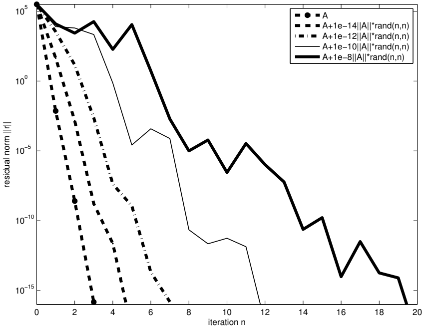
$\bar{Z}^T A \bar{Z} y = \bar{Z}^T b$, where $x = \bar{Z} y$

$\bar{U}$ approximates the Cholesky factor of $(Z^{(0)})^T A Z^{(0)}$

the loss of orthogonality $\|\bar{Z}^T A \bar{Z} - I\|$
the factorization error $\|Z^{(0)} - \bar{Z}\bar{U}\|$
Cholesky factorization error $\|(Z^{(0)})^T A Z^{(0)} - \bar{U}^T \bar{U}\|$



Problem 1a (inverse Hilbert matrix)
Loss of orthogonality ||I−Z^T AZ||
condition number (A)
∅= 0
∅= 1e−14
∅= 1e−12
∅= 1e−10
∅= 1e−8
u * ||A||||Z||^2||X^T X||
1e−14 * ||A||||Z||^2||X^T X||
1e−12 * ||A||||Z||^2||X^T X||
1e−10 * ||A||||Z||^2||X^T X||
1e−8 * ||A||||Z||^2||X^T X||



residual norm ||r||
iteration n
A
A+1e−14||A||*rand(n,n)
A+1e−12||A||*rand(n,n)
A+1e−10||A||*rand(n,n)
A+1e−8||A||*rand(n,n)

Eigenvalue based implementation - EIG

1. spectral decomposition $A = V\Lambda V^T$
2. QR factorization $\Lambda^{1/2}V^TZ^{(0)} = QU$
3. orthogonal-diagonal-orthogonal matrix multiplication $Z = V\Lambda^{-1/2}Q$

backward stable eigendecomposition + backward stable QR:

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

Gram-Schmidt orthogonalization

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

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

$$\alpha_{ji} = \langle z_i^{(j-1)}, z_j^{(0)} \rangle_A / \alpha_{jj}$$

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 MGS algorithm:

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

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

Loss of orthogonality in the CGS and AINV algorithms

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

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

Classical Gram-Schmidt (CGS2) with reorthogonalization

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

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

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

Local errors in the inner product and normalization

general positive definite A :

$$|\mathrm{fl}[\langle z_i^{(j-1)}, z_j\rangle_A] - \langle z_i^{(j-1)}, z_j\rangle_A| \leq \mathcal{O}(u)\|A\|\|z_i^{(j-1)}\|\|z_j\|$$
$$|1 - \|z_j\|_A^2| \leq \mathcal{O}(u)\|A\|\|z_j\|^2$$

diagonal (weight matrix) A :

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

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:

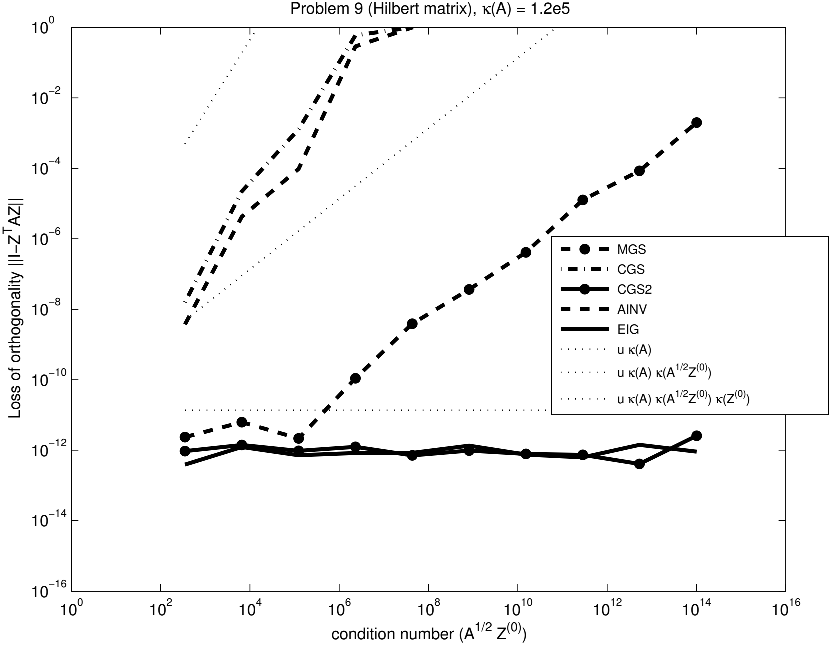
$$\mathcal{O}(u)\kappa(A^{1/2}Z^{(0)}) < 1$$

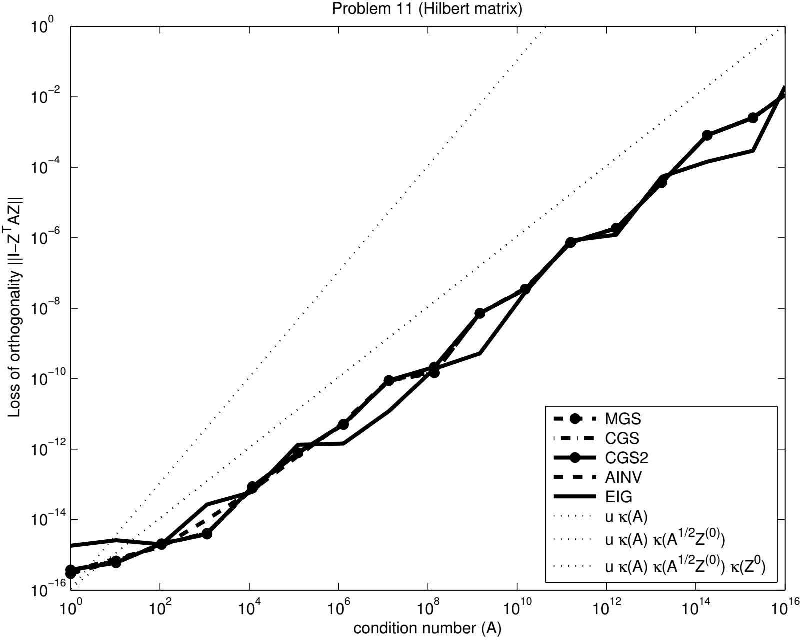
$$\|I - \bar{Z}^T A \bar{Z}\| \leq \mathcal{O}(u)$$

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

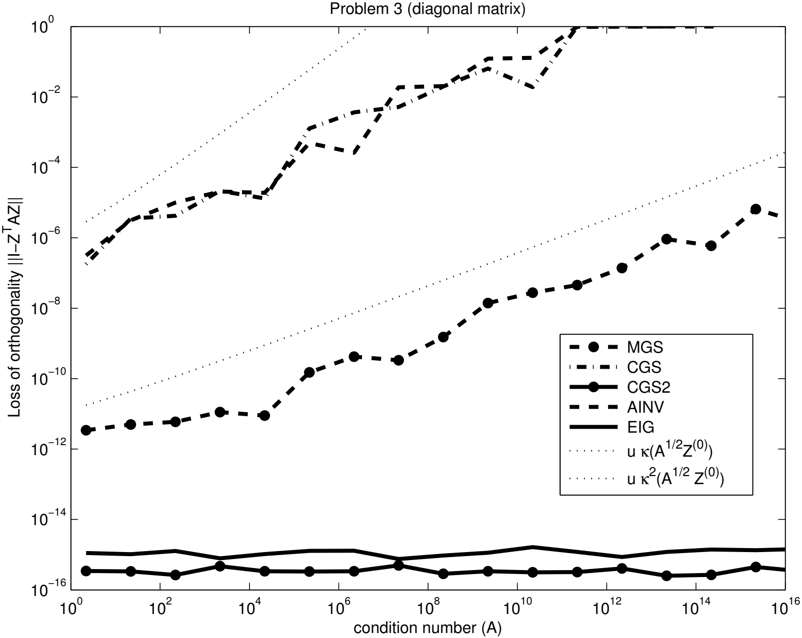
Numerical experiments - four extremal cases

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
4. $Z^{(0)} = I$

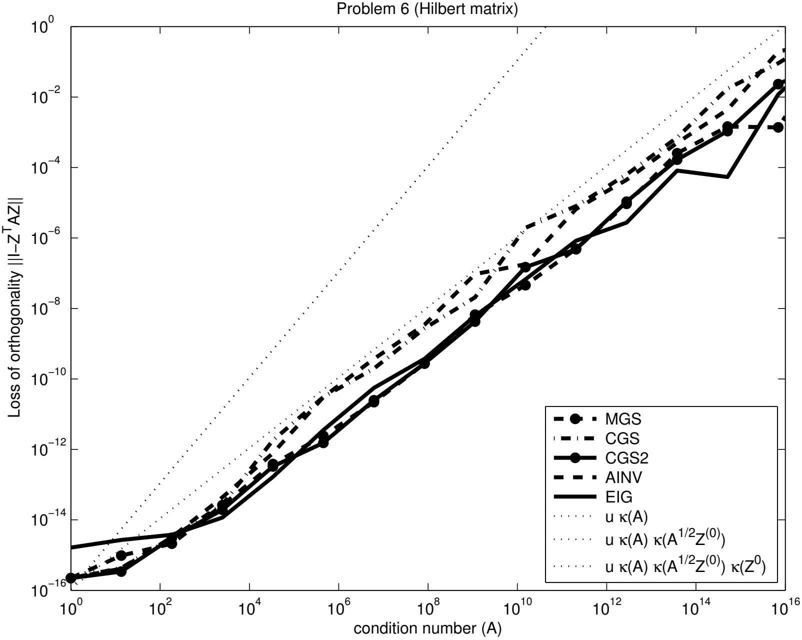

Problem 9 (Hilbert matrix), κ(A) = 1.2e5
Loss of orthogonality ||I−Z^T AZ||
condition number (A^{1/2} Z^{(0)})
MGS
CGS
CGS2
AINV
EIG
u κ(A)
u κ(A) κ(A^{1/2}Z^{(0)})
u κ(A) κ(A^{1/2}Z^{(0)}) κ(Z^{(0)})
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
10^0
10^2
10^4
10^6
10^8
10^10
10^12
10^14
10^16



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)
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
10^0
10^2
10^4
10^6
10^8
10^10
10^12
10^14
10^16
MGS
CGS
CGS2
AINV
EIG
u κ(A^1/2 Z^(0))
u κ^2(A^1/2 Z^(0))


Problem 6 (Hilbert matrix)
Loss of orthogonality ||I−Z^T AZ||
condition number (A)
10^0
10^−2
10^−4
10^−6
10^−8
10^−10
10^−12
10^−14
10^−16
10^0
10^2
10^4
10^6
10^8
10^10
10^12
10^14
10^16
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)

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.