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

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A symmetric positive definite $m \times m$ matrix

$Z^{(0)} = [z^{(0)}_1, \ldots, z^{(0)}_n]$ full column rank $m \times n$ matrix

$A$-orthogonal basis of $\text{span}(Z^{(0)})$: $Z = [z_1, \ldots, z_n]$ - $m \times n$ matrix

having orthogonal columns with respect to the inner product $\langle \cdot, \cdot \rangle_A$

$U$ upper triangular $n \times n$ matrix

\[
Z^{(0)} = ZU, \quad Z^T AZ = I
\]

\[
(Z^{(0)})^T AZ^{(0)} = U^T U
\]
\[
Z^T A Z = (A^{1/2} Z)^T (A^{1/2} Z) = I \implies \\
A^{1/2} Z \text{ is orthogonal with respect to the standard inner product} \\
A^{1/2} Z^{(0)} = (A^{1/2} Z) U \text{ is a standard QR factorization} \\
\kappa(Z) \ll \kappa^{1/2}(A) \\
\kappa(U) = \kappa(A^{1/2} Z^{(0)}) \leq \kappa^{1/2}(A) \kappa(Z^{(0)}) \\
\text{particular case } Z^{(0)} = I: Z = U^{-1} \text{ upper triangular } m \times n \text{ matrix} \\
\kappa(U) = \kappa(Z)
\]
Approximation properties of orthogonal factor

\[ Z^T AZ = I \]

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

\[ AZZ^T : \text{ orthogonal projector onto } R(AZ^{(0)}) \text{ and orthogonal to } R(Z^{(0)}) \]

\[ ZZ^T A : \text{ orthogonal projector onto } R(Z^{(0)}) \text{ and orthogonal to } R(AZ^{(0)}) \]

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

\[ ZZ^T = A^{-1} \]
Important application: approximate inverse preconditioning

\[ \tilde{Z} \] gives the approximate inverse \( \tilde{Z}\tilde{Z}^T \approx A^{-1} \]

\[ Ax = b \]

\[ \tilde{Z}^T A\tilde{Z} y = \tilde{Z}^T b \], where \( x = \tilde{Z} y \)

\( \tilde{U} \) approximates the Cholesky factor of \( (Z^{(0)})^T AZ^{(0)} \)

the loss of orthogonality \( \| \tilde{Z}^T A\tilde{Z} - I \| \)
the factorization error \( \| Z^{(0)} - \tilde{Z}\tilde{U} \| \)
Cholesky factorization error \( \| (Z^{(0)})^T AZ^{(0)} - \tilde{U}^T \tilde{U} \| \)
Problem 1a (inverse Hilbert matrix)

\[
\|I - ZTAZ\| \quad \text{condition number (A)}
\]

\[
\|A\| = 0
\]

\[
\|A\| = 1 \times 10^{-14}
\]

\[
\|A\| = 1 \times 10^{-12}
\]

\[
\|A\| = 1 \times 10^{-10}
\]

\[
\|A\| = 1 \times 10^{-8}
\]

\[
u \times \|A\| \times \|Z\|^2 \times \|XTX\|
\]

\[
1 \times 10^{-14} \times \|A\| \times \|Z\|^2 \times \|XTX\|
\]

\[
1 \times 10^{-12} \times \|A\| \times \|Z\|^2 \times \|XTX\|
\]

\[
1 \times 10^{-10} \times \|A\| \times \|Z\|^2 \times \|XTX\|
\]

\[
1 \times 10^{-8} \times \|A\| \times \|Z\|^2 \times \|XTX\|
\]
1. spectral decomposition $A = V\Lambda V^T$
2. QR factorization $\Lambda^{1/2}V^TZ^{(0)} = QU$
3. orthogonal-diagonal-orthogonal matrix multiplication $Z = VA^{-1/2}Q$

backward stable eigendecomposition + backward stable QR:

$$\|\tilde{Z}^TA\tilde{Z} - I\| \leq O(\nu)\|A\|\|\tilde{Z}\|^2$$
Gram-Schmidt orthogonalization

\[ z_i^{(j)} = z_i^{(j-1)} - \alpha_{ji} z_j \]

\[ z_i = \frac{z_i^{(i-1)}}{\alpha_{ii}}, \quad \alpha_{ii} = \|z_i^{i-1}\|_A \]

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

\[ \alpha_{ji} = \frac{\langle z_i^{(j-1)}, z_j^{(0)} \rangle_A}{\alpha_{jj}} \]
Local errors in the (modified) Gram-Schmidt process

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

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

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

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

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

\[ \langle z_i^{(j)}, z_j \rangle_A = \left( \text{fl}[\langle z_i^{(j-1)}, z_j \rangle_A] - \langle z_i^{(j-1)}, z_j \rangle_A \right) \| z_j \|_A^2 \]
Loss of orthogonality in the MGS algorithm:

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

\[ \|I - \tilde{Z}^T A \tilde{Z}\| \leq \frac{\mathcal{O}(u) \|A\| \|\tilde{Z}\|^2 \kappa(A^{1/2}Z^{(0)})}{1 - \mathcal{O}(u) \|A\| \|\tilde{Z}\|^2 \kappa(A^{1/2}Z^{(0)})} \]
Loss of orthogonality in the CGS and AINV algorithms

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

\[
\|I - \tilde{Z}^T A \tilde{Z}\| \leq \frac{O(u) \|A\|^{1/2} \|\tilde{Z}\| \kappa(A^{1/2}Z^{(0)}) \kappa^{1/2}(A) \kappa(Z^{(0)})}{1 - O(u) \|A\|^{1/2} \|\tilde{Z}\| \kappa(A^{1/2}Z^{(0)}) \kappa^{1/2}(A) \kappa(Z^{(0)})}
\]
Classical Gram-Schmidt (CGS2) with reorthogonalization

\[ z^{(1)}_i = z^{(0)}_i - \sum_{j=1}^{i-1} \alpha^{(1)}_{ji} z_j, \quad \alpha^{(1)}_{ji} = \langle z^{(0)}_i, z_j \rangle_A \]

\[ z^{(2)}_i = z^{(1)}_i - \sum_{j=1}^{i-1} \alpha^{(2)}_{ji} z_j, \quad \alpha^{(2)}_{ji} = \langle z^{(1)}_i, z_j \rangle_A \]

\[ z_i = z^{(2)}_i / \alpha_{ii}, \quad \alpha_{ii} = \| z^{(2)}_i \|_A \]

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

\[ \| I - \bar{Z}^T A \bar{Z} \| \leq O(u) \| A \| \| \bar{Z} \|^2 \]
Local errors in the inner product and normalization

general positive definite $A$:

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

$$|1 - \|z_j\|_A^2| \leq O(u)\|A\|\|z_j\|^2$$

diagonal (weight matrix) $A$:

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

$$|1 - \|z_j\|_A^2| \leq O(u)$$
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 - 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), $\kappa(A) = 1.2e5$

Loss of orthogonality $||I-Z^T AZ||$

Condition number $(A^{1/2} Z(0))$

Orthogonalization with a non-standard inner product

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Problem 11 (Hilbert matrix)

Loss of orthogonality $\|I - Z^T AZ\|

condition number (A)

MGS
CGS
CGS2
AINV
EIG

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

Orthogonalization with a non-standard inner product

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Orthogonalization with a non-standard inner product

Problem 3 (diagonal matrix)

Loss of orthogonality $\|I - Z^T A Z\|$
Problem 6 (Hilbert matrix)

Loss of orthogonality $||I-Z^T AZ||$

condition number (A)

MGS
CGS
CGS2
AINV
EIG

u κ(A)
κ(A 1/2Z(0)) κ(Z 0)

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Thank you for your attention!!!