Computation of the CS and the indefinite CS decomposition

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Introduction

Outline of the talk:

- definition of the CS and the hyperbolic CS decomposition,
- brief description of the known methods for the computation of the CSD,
- new Jacobi–type SVD algorithm for the computation of the CSD and the HCSD,
- implementation details,
- minor problems in the computational procedure.

Applications of the CSD

- used in computation of angles between subspaces, in rudimentary form known by Camille Jordan in 1875,
- rediscovered by Chandler Davis and William Kahan in 1969,
- stated in the Golub–Van Loan's textboox Matrix Analysis, 1983 in the context of angles beetwen subspaces, and distances between orthogonal projectors,
- used by Van Loan in construction of the generalized SVD,
- proof of the CSD given in Stewart–Sun's book Matrix Perturbation Theory, 1990,
- used by Vjeran Hari, 2005, to speed up the updates in the block–Jacobi SVD algorithm.

Definition of the CSD

Cosine Sine Decomposition (CSD)

- Let $Q \in \mathbb{C}^{n\times n}$ be a unitary matrix, partitioned as follows

$$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \begin{matrix} \leftarrow & k \\ \leftarrow & n-k \end{matrix}, \qquad 1 \le k \le n-1.$$
$$\begin{matrix} \uparrow & \uparrow \\ k & n-k \end{matrix}$$

- Then Q can be decomposed into three unitary matrices,

$$Q = U\Theta V^* = \begin{bmatrix} U_{11} & O \\ O & U_{22} \end{bmatrix} \Theta \begin{bmatrix} V_{11} & O \\ O & V_{22} \end{bmatrix}^*,$$

where U_{11} and V_{11} are square of order k, while U_{22} and V_{22} are square are of order $n-k$.

Definition of the CSD ctnd.

Matrix Θ

- If $2k \geq n$ then

$$\Theta = \left[\begin{array}{cc|c} I & & \\ & C & -S \\ \hline & S & C \end{array}\right] \begin{array}{l} \leftarrow 2k-n \\ \leftarrow n-k \\ \leftarrow n-k \end{array}$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ 2k-n & n-k & n-k \end{array}$$

- else if $2k \leq n$

$$\Theta = \left[\begin{array}{c|cc} C & & -S \\ \hline & I & \\ S & & C \end{array}\right] \begin{array}{l} \leftarrow k \\ \leftarrow n-2k \\ \leftarrow k \end{array}$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ k & n-2k & k \end{array}$$

C and S are real and diagonal, $C_{ii} \geq 0$, with nonincreasing diagonal, $S_{ii} \geq 0$ and $C^2 + S^2 = I$ holds.

Computation of the CSD

Brian Sutton's approach

- simultaneous bidiagonalization of the all four blocks,
- afterwards divide and conquer SVD on the bidiagonal matrices.

Vjeran Hari's approach

- compute the two SVD's of the diagonal blocks of the orthogonal matrix,
- clean-up of the offdiagonal blocks (in the case of multiple or close to multiple eigenvalues).

Definition of the Hyperbolic Cosine Sine Decomposition

Hyperbolic Cosine Sine Decomposition (HCSD)

- Let $Q \in \mathbb{C}^{n\times n}$ be a J–unitary matrix with respect to J, $J = \mathrm{diag}(I_k, -I_{n-k})$, i.e., $Q^* J Q = J$

$$Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \begin{matrix} \leftarrow & k \\ \leftarrow & n-k \end{matrix}, \qquad 1 \le k \le n-1.$$
$$\begin{matrix} \uparrow & & \uparrow \\ k & & n-k \end{matrix}$$

- Then Q can be factored into two (J–)unitary matrices U and V, and J–unitary matrix Θ

$$Q = U\Theta V^* = \begin{bmatrix} U_{11} & O \\ O & U_{22} \end{bmatrix} \Theta \begin{bmatrix} V_{11} & O \\ O & V_{22} \end{bmatrix}^*,$$

where U_{11} and V_{11} are square of order k, while U_{22} and V_{22} are square are of order $n-k$.

Definition of the HCSD (continued)

Matrix Θ

- If $2k \geq n$ then

$$\Theta = \left[\begin{array}{cc|c} C & & S \\ & I & \\ \hline S & & C \end{array}\right] \begin{array}{l} \leftarrow\ 2k-n \\ \leftarrow\ n-k \\ \leftarrow\ n-k \end{array}$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ 2k-n & n-k & n-k \end{array}$$

- else if $2k \leq n$

$$\Theta = \left[\begin{array}{c|cc} C & S & \\ \hline S & C & \\ & & I \end{array}\right] \begin{array}{l} \leftarrow\ k \\ \leftarrow\ k \\ \leftarrow\ n-2k \end{array}$$

$$\begin{array}{ccc} \uparrow & \uparrow & \uparrow \\ k & k & n-2k \end{array}$$

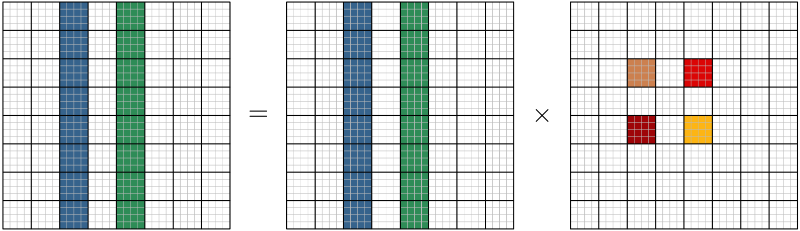
C and S are real and diagonal, $C_{ii} \geq 1$, with nonincreasing diagonal, $S_{ii} \geq 0$ and $C^2 - S^2 = I$ holds.

Applications of the HCSD

- derived in the PhD. thesis of Ninoslav Truhar,
- used in computation of the singular values of a J-unitary matrix,
- computation of the 2-norm of a J-unitary matrix,
- bounds for the hyperbolic sine of the maximal hyperbolic cannonical angle,
- tool to speed up the updates in the hyperbolic block–Jacobi SVD algorithm.

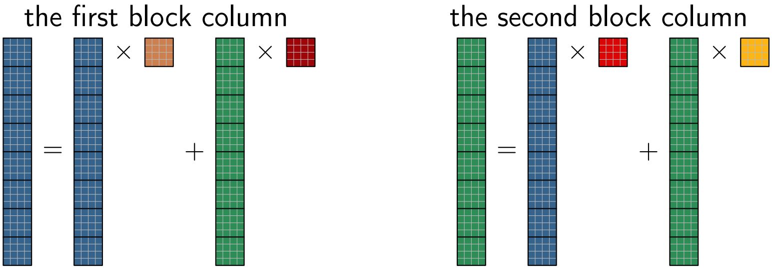
Updates in the (hyperbolic) Block Jacobi SVD algorithm

Update of the factor after the block transformation



Columnwise updates

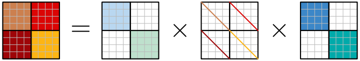
Update of the factor after the block transformation



Columnwise updates

Update of the factor after the block transformation (HCSD)

HCSD of the block-rotation



- at the first step, postponed matrix V^T is I,
- multiply part of the postponed block diagonal matrix V^T by the current matrix U from the current HCSD,
- multiply the first and the second block column by the appropriate $V^T U$,
- apply `xAXPY`–like in-place operation (multiplication by the CS matrix),
- postpone last matrix V^T of the current HCSD to the new step.

Properties of the HCSD

Proposition 1

If Q is J-unitary, and J satisfies $J^2 = I$, then Q^* is also J-unitary.

Proof

- By definition Q is nonsingular.
- Multiplication of $Q^* JQ = J$, by QJ from the left, and by $Q^{-1}J$ from the right completes the proof. $\square$

Properties of the HCSD (continued)

Proposition 2

If Q is is J-unitary and partitioned according to signs of the diagonal elements in J, and $U, V \in \mathbb{C}^{n \times n}$ are unitary block-matrices

$$U = \operatorname{diag}(U_{kk}, U_{n-k,n-k}), \quad V = \operatorname{diag}(V_{kk}, V_{n-k,n-k}),$$

then W, where $W = U^* Q V$, remains J-unitary.

Proof

- Due to block structure of U and V, they are both J-unitary matrices.
- Then, it follows

$$W^* J W = V^* Q^* U J U^* Q V = V^* Q^* J Q V = V^* J V = J. \qquad \square$$

SVD and the structure of the blocks

SVDs of the diagonal blocks or SVDs of the off-diagonal blocks?

- If $k \neq n - k$ then the SVDs of the off-diagonal blocks can be computed faster (suppose that $k < n - k$):
  - QR factorization of the block Q_{21} followed by the SVD of the matrix of order k,
  - LQ factorization of the block Q_{12} followed by the SVD of the matrix of order k

  versus
  - SVD of the matrix of order k,
  - SVD of the matrix of order $n - k$.
- Since $C_{ii} > S_{ii}$ in the hyperbolic case, it is more accurate to determine to high relative accuracy smaller of the quantities, i.e., matrix S!

SVD and the structure of the blocks

Structures of the blocks

- Suppose that SVDs of Q_{12} and Q_{21} are computed,

$$Q_{12} := U_{12} S_{12} V_{12}^* = U_{12} \begin{bmatrix} \Sigma & 0 \\ 0 & 0 \end{bmatrix} V_{12}^*, \quad \Sigma = \operatorname{diag}(\gamma_1, \ldots, \gamma_\ell),$$
$$\gamma_1 \geq \gamma_2 \geq \cdots \geq \gamma_\ell > 0,$$
$$Q_{21} := U_{21} S_{21} V_{21}^* = U_{21} \begin{bmatrix} \Sigma' & 0 \\ 0 & 0 \end{bmatrix} V_{21}^*, \quad \Sigma' = \operatorname{diag}(\gamma_1, \ldots, \gamma'_{\ell'}),$$
$$\gamma'_1 \geq \gamma'_2 \geq \cdots \geq \gamma'_{\ell'} > 0.$$

- Then W and W^*,

$$W := \begin{bmatrix} U_{12}^* & \\ & U_{21}^* \end{bmatrix} \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22} \end{bmatrix} \begin{bmatrix} V_{12} & \\ & V_{21} \end{bmatrix} = \begin{bmatrix} W_1 & S_{12} \\ S_{21} & W_2 \end{bmatrix}$$

are J-unitary.

Structures of the blocks

- If the partition of W_1 and W_2 are written according to the structures od S_{12} and S_{21}, we obtain

$$W = \left[\begin{array}{cc|cc} W_{11} & W_{12} & \Sigma & 0 \\ W_{21} & W_{22} & 0 & 0 \\ \hline \Sigma' & 0 & W_{33} & W_{34} \\ 0 & 0 & W_{43} & W_{44} \end{array}\right] \begin{array}{l} \leftarrow \ \ell \\ \leftarrow \ k-\ell \\ \leftarrow \ \ell' \\ \leftarrow \ n-k-\ell' \end{array}$$
$$\begin{array}{cccc} \uparrow & \uparrow & \uparrow & \uparrow \\ \ell' & k-\ell' & \ell & n-k-\ell \end{array}$$

- and by using that both W and W^* are J-unitary . . .

SVD and the structure of the blocks

Properties of the matrix W

- ... from $W^* J W = J$ we obtain the following set of equations:

$$
\begin{aligned}
W_{11}^* W_{11} - W_{21}^* W_{21} - (\Sigma')^2 &= I_{\ell'} \\
W_{12}^* W_{12} + W_{22}^* W_{22} &= I_{k-\ell'} \\
W_{33}^* W_{33} + W_{43}^* W_{43} - \Sigma^2 &= I_{\ell} \\
W_{34}^* W_{34} + W_{44}^* W_{44} &= I_{n-k-\ell} \\
W_{11}^* W_{12} + W_{21}^* W_{22} &= 0_{\ell', k-\ell'} \\
W_{11}^* \Sigma - \Sigma' W_{33} &= 0_{\ell', \ell} \\
\Sigma' W_{34} &= 0_{\ell', n-k-\ell} \\
W_{12}^* \Sigma &= 0_{k-\ell', \ell} \\
W_{33}^* W_{34} + W_{43}^* W_{44} &= 0_{\ell, n-k-\ell}
\end{aligned}
$$

SVD and the structure of the blocks

Structure of SVD the matrix W

- ... and from $WJW^* = J$:

$$
\begin{aligned}
W_{11}W_{11}^* - W_{12}W_{12}^* - \Sigma^2 &= I_\ell \\
W_{21}W_{21}^* + W_{22}W_{22}^* &= I_{k-\ell} \\
W_{33}W_{33}^* + W_{34}W_{34}^* - (\Sigma')^2 &= I_{\ell'} \\
W_{43}W_{43}^* + W_{44}W_{44}^* &= I_{n-k-\ell'} \\
W_{11}W_{21}^* + W_{12}W_{22}^* &= 0_{\ell,k-\ell} \\
W_{11}\Sigma' - \Sigma W_{33}^* &= 0_{\ell,\ell'} \\
\Sigma' W_{43}^* &= 0_{\ell,n-k-\ell'} \\
W_{21}^*\Sigma' &= 0_{k-\ell,\ell'} \\
W_{33}W_{43}^* + W_{34}W_{44}^* &= 0_{\ell',n-k-\ell'}.
\end{aligned}
$$

SVD and the structure of the blocks

After a simple manipulation, we have

- $W_{12} = 0_{\ell,k-\ell'}$, $W_{34} = 0_{\ell',\ell}$, $W_{21} = 0_{k-\ell,\ell'}$, $W_{43} = 0_{k-\ell',k-\ell}$,
- $\ell = \ell'$, $\Sigma = \Sigma'$,
- W_{22} and W_{44} are unitary matrices (and can be pulled out),
- $W_{33} = W_{11}^*$,
- W_{11} is a scaled unitary matrix, i.e.,

$$W_{11}^* W_{11} = W_{11} W_{11}^* = \Sigma^2 + I_\ell,$$

- moreover W_{11} has inner block structure

$$W_{11} = \mathrm{diag}(Z_1, \ldots, Z_q),$$

where each block Z_i corresponds to a possibly multiple singular value γ_i.

The algorithm for the HCSD

Algorithm for $k \leq n-k$

do in parallel

{compute the RR QR factorization of Q_{12}

compute the RR LQ factorization of Q_{21}}

do in parallel

{update U_{22} and V_{22}^*}

do (possibly) in parallel

{compute the SVDs of Q_{12} and Q_{21}}

do in parallel

{update matrices U and V^*}

if $n-k > k$ then

{extract the unitary block that corresponds to I in Q_{22}}

cleanup in parallel of the diagonal blocks in the case of multiple hyperbolic singular values

The parallel Jacobi SVD

Speed of the HCSD algorithm

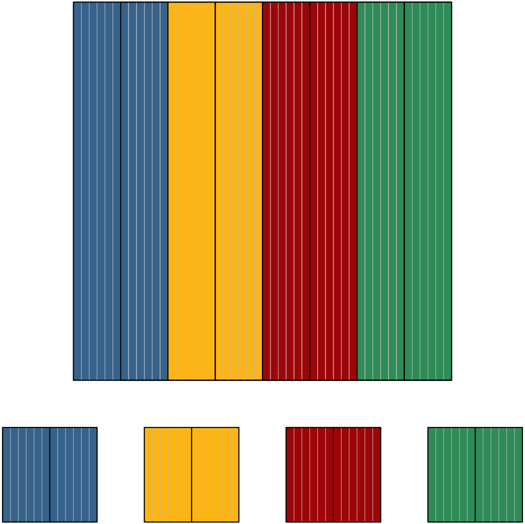
- almost exclusively depends on the speed of the SVD
- in addition, there are only few xGEMMs.

Multilevel Jacobi-type SVD algorithm

- can have 3 or 4 levels:
  - the first level targets L1 cache,
  - the second level targets multiple threads of one core,
  - the third level targets one NUMA domain,
  - possible fourth (MPI) level targets multiple machines.

The parallel Jacobi SVD

Levels of hierarchy



The parallel Jacobi SVD

The first level algorithm

- uses Advanced Vector eXtensions (AVXn) registers to process multiple doubles simultaneously, i.e., the algorithm process multiple independent columns in parallel

The main problem

- how to allocate appropriate number of threads for each level of the algorithm (work in progress).

Numerical testing

Test data

- matrices C, S, U and V are generated and multiplied in higher precision,
- resulting matrix is rounded to double precision.

Full testing

- is in progress.