

New Class of Block Matrix Orderings for the Parallel Two-Sided Jacobi SVD Algorithm

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Outline

New Block Orderings

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Problem formulation

Parallel Two-Sided Block-Jacobi Algorithm

Known Types of Block Ordering

New Clique-Based Block Ordering

First numerical results

- 1 Problem formulation
- 2 Parallel Two-Sided Block-Jacobi Algorithm
- 3 Known Types of Block Ordering
- 4 New Clique-Based Block Ordering
- 5 First numerical results

Our task

Compute in parallel the Singular Value Decomposition (SVD) of a complex matrix A of the size $m \times n$, $m \geq n$:

$$A = U \begin{pmatrix} \Sigma \\ 0 \end{pmatrix} V^H.,$$

where $U(m \times m)$ and $V(n \times n)$ are orthogonal and $\Sigma = \text{diag}(\sigma_i)$ with $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_n$.

Numerically stable way of computation:

- one- or two-sided block-Jacobi methods;
- large degree of parallelism.

Target architecture:

- distributed memory machines (parallel supercomputers and clusters) with Message Passing Interface (MPI).

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Known Types of Block Ordering

New Clique-Based Block Ordering

First numerical results

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- Implemented on p processors, an even blocking factor $\ell = 2p$ is used together with some ordering of subproblems.
- Each processor contains 2 block columns of A , U , V .
- Algorithm is based on the SVDs of 2×2 -block subproblems:

$$S_{ij} = \begin{pmatrix} A_{ij} & A_{ij} \\ A_{ji} & A_{ji} \end{pmatrix}.$$

- Global termination criterion:

$$F(A, \ell) = \sqrt{\sum_{i,j=1, i \neq j}^{\ell} \|A_{ij}\|_F^2} < \epsilon, \quad \epsilon \equiv \text{prec} \cdot \|A\|_F.$$

New Block Orderings

Gabriel Okša

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Parallel Two-Sided Block-Jacobi Algorithm

Known Types of Block Ordering

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Problem formulation

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Known Types of Block Ordering

New Clique-Based Block Ordering

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Problem formulation

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Known Types of Block Ordering

New Clique-Based Block Ordering

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$$F(\mathbf{S}_{ij}, \ell) = \sqrt{\|\mathbf{A}_{ij}\|_{\mathbb{F}}^2 + \|\mathbf{A}_{ji}\|_{\mathbb{F}}^2} < \delta, \quad \delta \equiv \epsilon \cdot \sqrt{\frac{2}{\ell(\ell-1)}}.$$

- **Main question:** How to order 2×2 -block subproblems to be efficient?

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Known Types of Block Ordering

New Clique-Based Block Ordering

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New Clique-Based Block Ordering

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- Let the matrix A be cut into $\ell \times \ell$ block structure with $\ell = 2p$ where p is the number of processors..
- **Cyclic block-row ordering** define 2×2 block subproblems by block rows:
 $(A_{12}, A_{21}), (A_{13}, A_{31}), \dots, (A_{1\ell}, A_{\ell 1}),$
 $(A_{23}, A_{32}), (A_{24}, A_{42}), \dots, (A_{2\ell}, A_{\ell 2}),$
 $\dots, (A_{\ell-1,\ell}, A_{\ell,\ell-1}).$
- **Cyclic bloc-column ordering** is defined similarly.
- **Parallel method:** Take p consecutive pairs from the list, each pair defines one 2×2 -block SVD subproblem for one processor.

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Problem formulation

Parallel Two-Sided Block-Jacobi Algorithm

Known Types of Block Ordering

New Clique-Based Block Ordering

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- During one **sweep** of the method each non-diagonal block of A is nullified exactly once.
- **Main problem:** The ordering is prescribed and fixed, there is no consideration about an *actual status* (e.g., Frobenius norm) of individual blocks—may be **very unefficient** in decreasing the off-norm.
- Significant amount of data (e.g., whole column blocks) need to be explicitly transferred among processors at the beginning of each parallel step.

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Known Types of Block Ordering

New Clique-Based Block Ordering

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New Block Orderings

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Problem formulation

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Known Types of Block Ordering

New Clique-Based Block Ordering

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- **Main idea:** Take into consideration the actual status of a matrix and, in one parallel iterations step (p subproblems) *decrease the off-norm as much as possible*.
- This task can be translated into the language of graph theory:
 - 1 Construct the weighted complete graph \mathcal{G} with ℓ vertices ($\ell = 2p$ is the blocking factor), where the edge (i, j) has the weight $\|A_{ij}\|_F^2 + \|A_{ji}\|_F^2$.
 - 2 At the beginning of each parallel iteration step, find the **maximum-weight perfect matching** on \mathcal{G} , which defines the p SVD subproblems—only *polynomial* complexity $O(\ell^3)$.

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New Block Orderings

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New Block Orderings

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New Clique-Based Block Ordering

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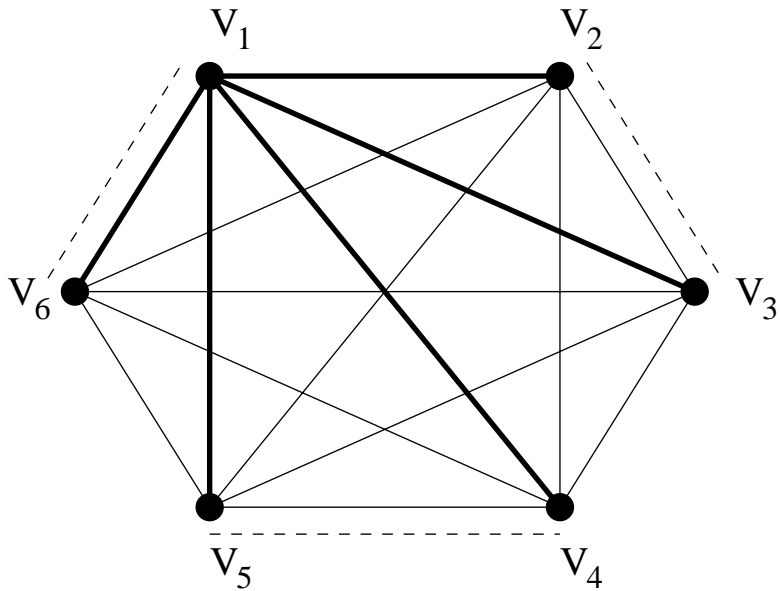


Figure: Maximum-weight perfect matching for $\ell = 6$ ($p = 3$).

Clique-Based Block Ordering

New Block Orderings

Gabriel Okša

Problem formulation

Parallel Two-Sided Block-Jacobi Algorithm

Known Types of Block Ordering

New Clique-Based Block Ordering

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- **Physical blocking factor**: for p processors, let A be partitioned into p block columns and block rows, each processor contains one block column.
- **Logical blocking factor**: $\ell = p/r$ for some integer r .
- In each parallel iteration step, ℓ local SVDs are computed in parallel where each SVD is of block-order $r \times r$ and comprises $2r$ off-diagonal blocks of A .
- **Our aim**: Decrease the off-diagonal Frobenius norm in each parallel iteration step as much as possible.

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New Block Orderings

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Known Types of Block Ordering

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- **Task:** Partition \mathcal{G} into $\ell/2$ disjoint cliques of size r where the weight of cliques (i.e., the sum of weights through the edges belonging to chosen cliques) is maximized.
- For $r = 2$ this is just the maximum-weight perfect matching used in the Dynamic Ordering.
- **Main problem:** For $r \geq 3$, this task is **NP-hard**.

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Problem formulation

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New Block Orderings

Gabriel Okša

Problem formulation

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Known Types of Block Ordering

New Clique-Based Block Ordering

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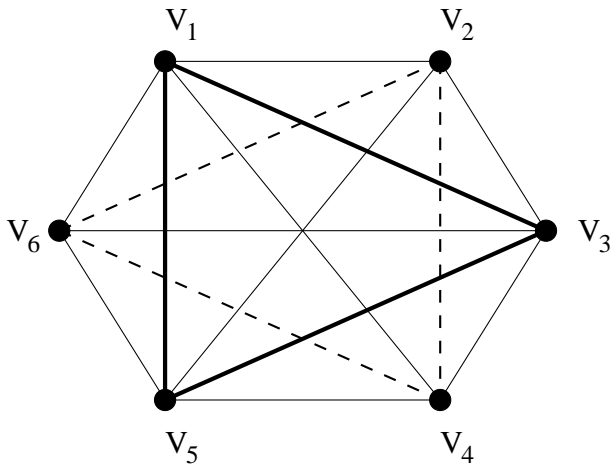
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CLIQUE 1: INDICES (1, 3, 5) (blocks and processors)

CLIQUE 2: INDICES (2, 4, 6) (blocks and processors)

Figure: Clique-based block ordering for $p = 6$, $r = 3$.

Example (cont.)

- In the example above there are 2 local SVDs defined by submatrices with block indices (1, 3, 5) and (2, 4, 6):

$$\text{CL1} = \begin{pmatrix} A_{11} & A_{13} & A_{15} \\ A_{31} & A_{33} & A_{35} \\ A_{51} & A_{53} & A_{55} \end{pmatrix}, \quad \text{CL2} = \begin{pmatrix} A_{22} & A_{24} & A_{26} \\ A_{42} & A_{44} & A_{46} \\ A_{62} & A_{64} & A_{66} \end{pmatrix}.$$

- **MPI library:** The SVD of CL1 is computed in the **context** that consists of processors 1, 3 and 5. Similarly, the SVD of CL2 is computed in the **context** that consists of processors 2, 4 and 6.
- In general, there are ℓ contexts, each with r processors.
- **Important:** The matrix data is **not moved explicitly** between processors at the beginning of a parallel iteration step—just new contexts are created.

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First numerical results

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- 1 Given p , r , ℓ and actual weights $\|A_{ij}\|_F^2 + \|A_{ji}\|_F^2$, find ℓ maximum-weight disjoint cliques using **a genetic serial algorithm** in processor 1—this defines the new block ordering.
- 2 Broadcast the new block ordering to all processors.
- 3 Delete old contexts.
- 4 Create ℓ contexts based on the new ordering, each context of size r , and compute ℓ SVDs of block size $r \times r$ in parallel by the two-sided Jacobi method.
- 5 Update left and right singular vectors in all processors by matrix multiplications.
- 6 Update weights $\|A_{ij}\|_F^2 + \|A_{ji}\|_F^2$.

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New Block Orderings

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Known Types of Block Ordering

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- 1 Given p , r , ℓ and actual weights $\|A_{ij}\|_F^2 + \|A_{ji}\|_F^2$, find ℓ maximum-weight disjoint cliques using **a genetic serial algorithm** in processor 1—this defines the new block ordering.
- 2 Broadcast the new block ordering to all processors.
- 3 Delete old contexts.
- 4 Create ℓ contexts based on the new ordering, each context of size r , and compute ℓ SVDs of block size $r \times r$ in parallel by the two-sided Jacobi method.
- 5 Update left and right singular vectors in all processors by matrix multiplications.
- 6 Update weights $\|A_{ij}\|_F^2 + \|A_{ji}\|_F^2$.

Work in one parallel iteration step

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Gabriel Okša

Problem formulation

Parallel Two-Sided Block-Jacobi Algorithm

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Genetic algorithm

- The serial genetic algorithm for the maximum-weight clique partition has been implemented in C++ using the free available library `GALIB` (v. 2.4.6) from MIT, USA.
- The **genome** is the 2D binary string of dimensions $\ell \times p$ that represents one partition into disjoint cliques.
- The **crossover** function creates two new genomes (son and daughter) from two old genomes (parents) by choosing the heavier individual cliques (better parent is repeated).
- The **objective** function, which should be maximized, is the weight of a genome.
- Typical run:
population size = 20,
number of generations = 10^4 .

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Table: Performance for $p = 12$, $prec = 10^{-13}$, $\kappa = 10$, multiple minimal SV. T_p is in seconds, $R_{GA} = (T_{GA}/T_p) * 100$.

n	2 cliques			6 cliques		
	n_{iter}	T_p	R_{GA}	n_{iter}	T_p	R_{GA}
1000	37	98.8	4.3	409	866.1	7.5
2000	39	463.5	1.0	416	1544.8	4.2
3000	38	1393.3	0.3	406	3922.6	1.6
4000	36	3084.8	0.1	402	8054.4	0.8
5000	37	6144.0	0.1	403	15101.6	0.4
6000	37	9994.2	< 0.1	427	25951.0	0.2
7000	37	15926.5	< 0.1	412	39925.8	0.2
8000	35	23757.1	< 0.1	423	61874.0	0.1
9000	37	34040.0	< 0.1	417	85072.0	< 0.1
10000	38	56532.5	< 0.1	431	125658.6	< 0.1