

Computing the Rank Profile Matrix

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joint work with Jean-Guillame Dumas and Ziad Sultan

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Saclay, November 16, 2015.

Gaussian elimination in computer algebra

Swiss army knife for applications:

Matrix factorization

(LU decomposition)

- ▶ Solving linear systems
- ▶ Computing determinants

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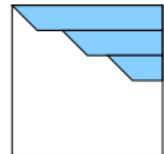
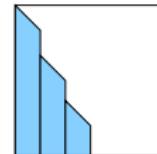
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Computing linear dependencies

(Echelon structure)

- ▶ Basis of vector spaces (Krylov iteration)
- ▶ Echelon structure of the Macaulay matrix
(Gröbner basis)



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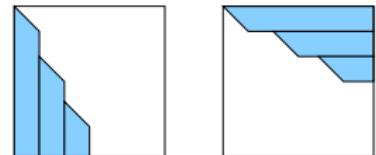
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(Echelon structure)



Rank profiles: how to select the first 3 linearly indep rows of

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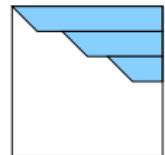
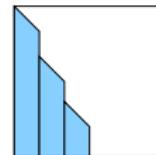
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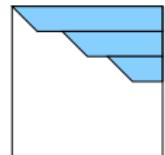
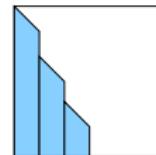
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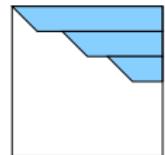
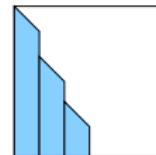
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Rank profiles

Definition (Row Rank Profile: RowRP)

Given $A \in \mathbb{K}^{m \times n}$, $r = \text{rank}(A)$.

informally: *first r* linearly independent rows

formally: lexico-minimal list of r indices of linearly independent rows.

Example

$$\begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

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Definition (Column Rank Profile: ColRP)

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Generic Rank Profile: first r leading principal minors $\neq 0$

Generic rank profile \Leftrightarrow Generic Row RP and Generic ColRP

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RowRP = ColRP = {1,2}

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RowRP = ColRP = {1,2}

But $|A_{1,1}| = 0$

Relation to echelon forms

Transformation to echelon form

$\forall A \exists X$ non-singular s.t.

$$\begin{matrix} X & \end{matrix} \quad \begin{matrix} A & = & R \end{matrix}$$

Relation to echelon forms:

- ▶ ColRP unchanged by left multiplication with an invertible matrix

ColRP = pivot columns in the **row** echelon form

Triangular Matrix decompositions and rank profiles

Decomposition	Exists for	Unique
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$$\begin{matrix} A \\ = \\ L \end{matrix} \quad \begin{matrix} U \end{matrix}$$

Generic rank profile



Triangular Matrix decompositions and rank profiles

Decomposition	Exists for	Unique
$A = L U$	Generic rank profile	✓
$A = L U P$	Generic row rank profile	✗
$A = P L U$	Generic col rank profile	✗

Triangular Matrix decompositions and rank profiles

Decomposition	Exists for	Unique
$A = L \cdot U$	Generic rank profile	✓
$A = L \cdot U \cdot P$	Generic row rank profile	✗
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$A = P \cdot L \cdot U \cdot Q$	Any matrix	✗

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→ P, Q may reveal row and/or col rank profiles.

Computing rank profiles

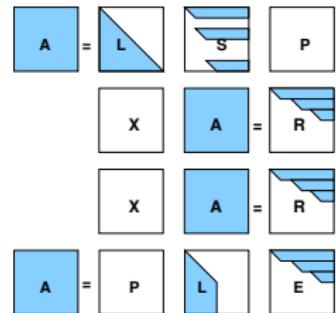
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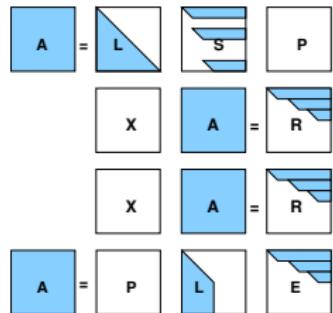
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Lessons learned (or what we thought was necessary):

- ▶ treat rows in order
- ▶ exhaust all columns before considering the next row
- ▶ **slab** block splitting (recursive or iterative)
- ~~ similar to partial pivoting



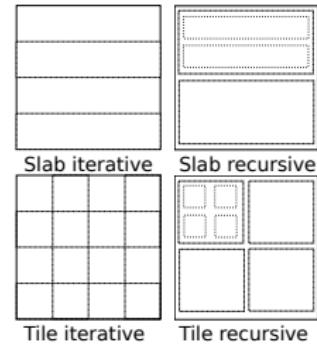
Motivation

Need more flexible blocking

Slab blocking

- ▶ leads to inefficient memory access patterns
- ▶ is harder to parallelize

Tile blocking instead ?



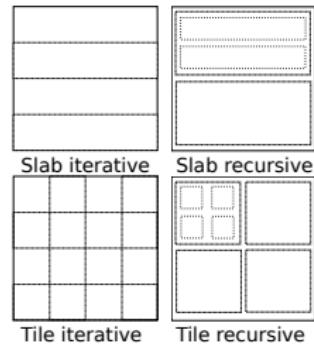
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Gathering linear independence invariants

Two ways to look at a matrix (looking left or right):

- ▶ Row rank profile, column echelon form
- ▶ Column rank profile, row echelon form

Unique invariant?

Outline

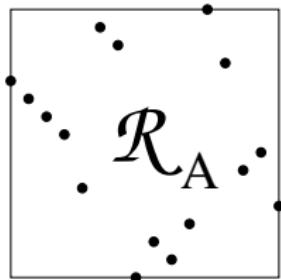
- 1 The rank profile Matrix
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- 4 Relations to other decompositions
- 5 Generalization over a Ring
- 6 The small rank case

The rank profile Matrix

Theorem

Let $A \in \mathbb{F}^{m \times n}$.

There exists a *unique*, $m \times n$, $\text{rank}(A)$ -sub-permutation matrix \mathcal{R}^A of which every leading sub-matrix has the same rank as the corresponding leading sub-matrix of A .



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Example

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Properties of the rank profile matrix

Properties

- A invertible $\Rightarrow \mathcal{R}^A$ is a permutation matrix
- A is square with generic rank profile $\Rightarrow \mathcal{R}^A = I_n$
- $\text{RowRP}(A) = \text{RowSupport}(\mathcal{R}^A)$
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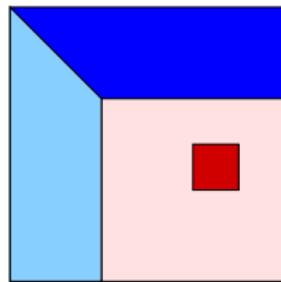
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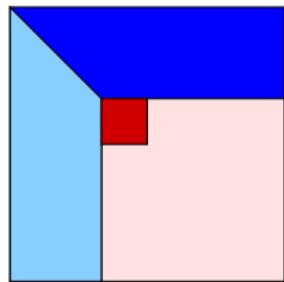
Anatomy of a PLUQ decomposition



Four types of elementary operations:

Search: finding a pivot

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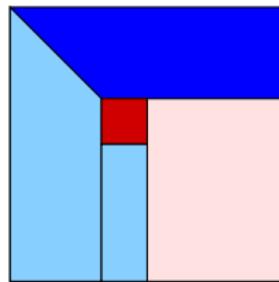


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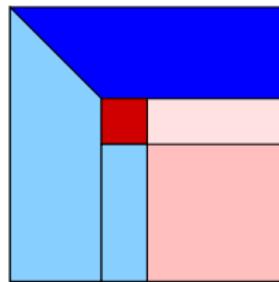
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Normalization: computing L : $l_{i,k} \leftarrow \frac{a_{i,k}}{a_{k,k}}$

Update: applying the elimination $a_{i,j} \leftarrow a_{i,j} - \frac{a_{i,k}a_{k,j}}{a_{k,k}}$

Impact on the PLUQ decomposition

Normalization: determines whether L or U is unit diagonal

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Problem (Reformulation)

*Under what conditions on the **Search** and **Permutation** operations does a PLUQ decomposition algorithm reveals RowRP, ColRP or \mathcal{R}^A ?*

The Pivoting matrix

Definition (The pivoting matrix)

Given a PLUQ decomposition $A = PLUQ$ with rank r , define

$$\Pi_{P,Q} = P \begin{bmatrix} I_r \\ 0 \end{bmatrix} Q.$$

Locates the position of the pivots in the matrix A .

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- ▶ $\text{RowSupp}(\Pi_{P,Q}) = \text{RowSupp}(\mathcal{R}^A) = \text{RowRP}(A)$ (*Weaker*)
- ▶ $\text{ColSupp}(\Pi_{P,Q}) = \text{ColSupp}(\mathcal{R}^A) = \text{ColRP}(A)$ (*Weaker*)

The Search operation

Various strategies depending on the context

Numerical stability: find the absolute largest pivot

Data locality: find pivot not too far from the main diagonal

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Search revealing rank profiles

- ▶ No stability issue over exact domains
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Example

Search: “Any non zero element on the topmost row”:

$$A = \begin{bmatrix} 2 & 0 & 3 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 2 & 0 & 1 \end{bmatrix} \Rightarrow \mathcal{R}^A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$

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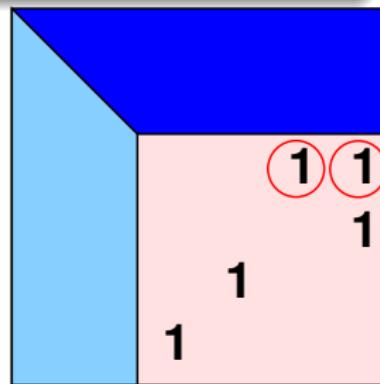
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Pivoting and permutation strategies

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Pivot's (i, j) position minimizes some pre-order:

Row order: any non-zero on the first non-zero row

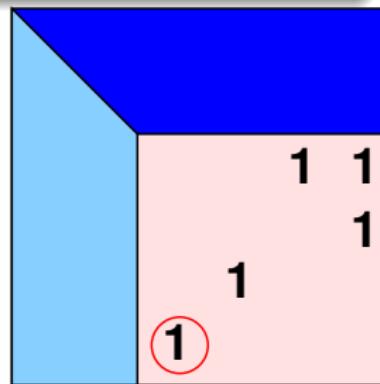


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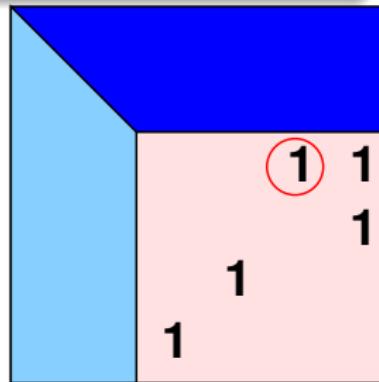
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Lex order: first non-zero on the first non-zero row



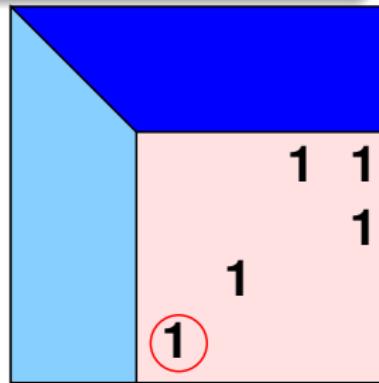
Pivoting and permutation strategies

Pivot Search

Pivot's (i, j) position minimizes some pre-order:

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Pivoting and permutation strategies

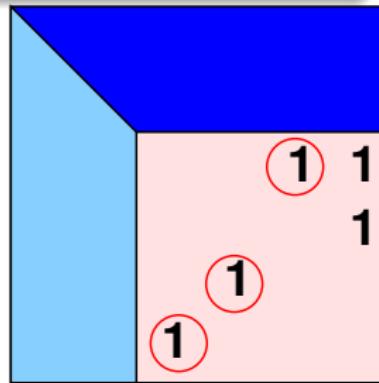
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Sufficient ?

Is lexicographic ordering sufficient to reveal both rank profiles?

Example

With a lexicographic ordering

$$\textcircled{1} \quad A = \begin{bmatrix} 2 & 0 & 3 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 4 & 0 \\ 0 & 2 & 0 & 1 \end{bmatrix} \Rightarrow \mathcal{R}^A = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} = \Pi_{P,Q}$$

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- ~~~ Pivot Swaps mix-up precedence between rows/cols.
- ~~~ **Permutations** also have to be considered

Pivoting and permutation strategies

Pivot Search

Pivot's (i, j) position minimizes some pre-order:

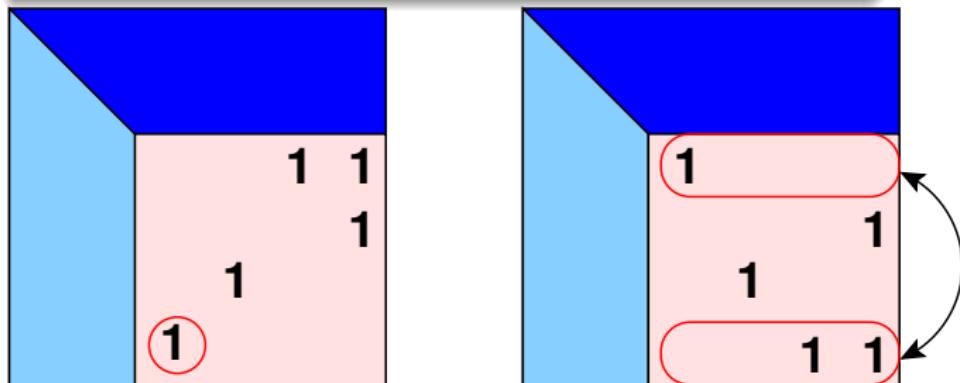
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Permutation

- ▶ Transpositions



Transposition

Pivoting and permutation strategies

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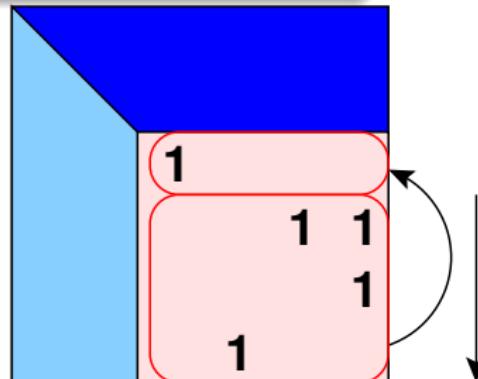
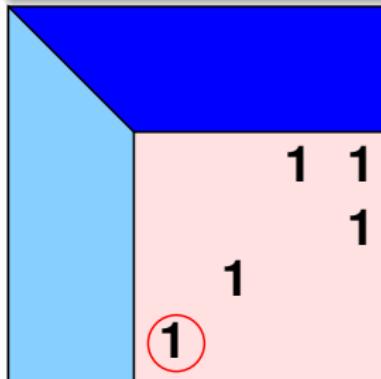
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Permutation

- ▶ Transpositions
- ▶ Cyclic Rotations



Cyclic rotation

Pivoting strategies revealing rank profiles

For any type of PLUQ algorithm: iterative / block iterative / recursive

Search	Row perm.	Col. perm.	RowRP	ColRP	\mathcal{R}^A	Instance
Row order						
Col. order						
Lexico.						
Rev. lex.						
Product						

Pivoting strategies revealing rank profiles

For any type of PLUQ algorithm: iterative / block iterative / recursive

Search	Row perm.	Col. perm.	RowRP	ColRP	\mathcal{R}^A	Instance
Row order Col. order	Transposition	Transposition	✓			[IMH82] [JPS13]
Lexico.						
Rev. lex.						
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- $\text{RowRP} = [1 \ 2 \ \dots \ m] P \begin{bmatrix} I_r \\ 0 \end{bmatrix}$

Pivoting strategies revealing rank profiles

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Product	Rotation	Rotation	✓	✓	✓	[DPS13]

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Lexico.	Rotation	Rotation	✓	✓	✓	[DPS15]
Rev. lex.	Transposition	Transposition		✓		[Sto00]
Rev. lex.	Rotation	Transposition	✓	✓	✓	[DPS15]
Rev. lex.	Rotation	Rotation	✓	✓	✓	[DPS15]
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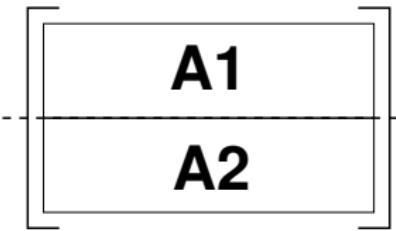
Outline

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The slab recursive algorithm

Slab Recursive LU [IMH82, KG85, Sto00, JPS13]

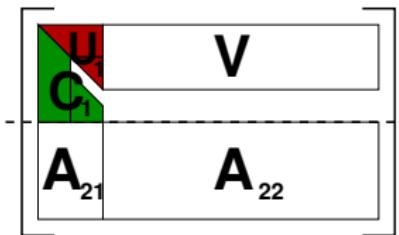
- ➊ Split A Row-wise



The slab recursive algorithm

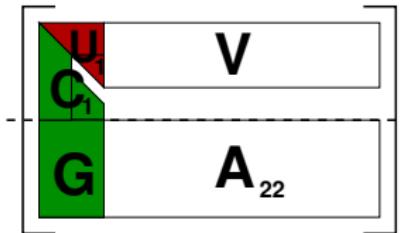
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The slab recursive algorithm

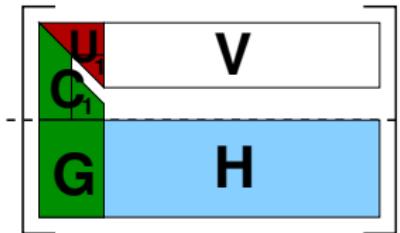
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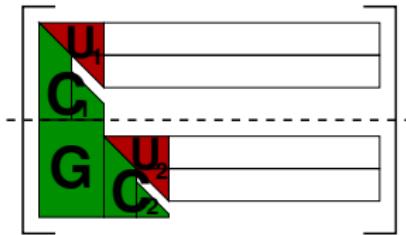
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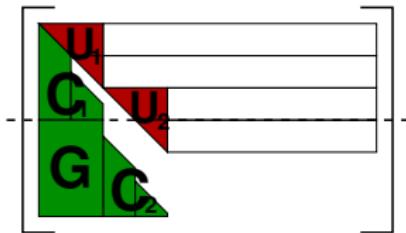
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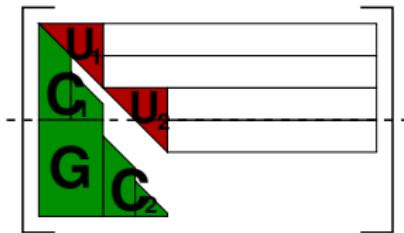
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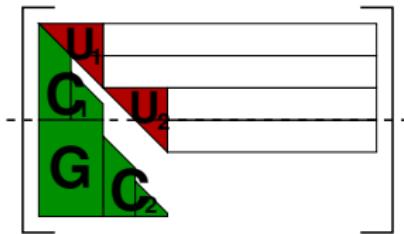
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Implements the lexicographic order search.

- ▶ Col/Row Transpositions : Computes the ColRP

The slab recursive algorithm

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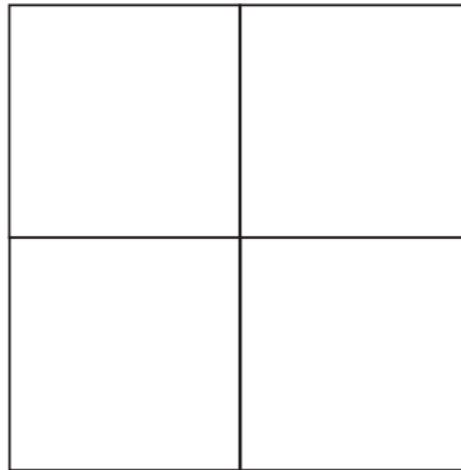
Implements the lexicographic order search.

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- ▶ Row Rotations : Computes \mathcal{R}^A [DPS15]

The tiled recursive algorithm



Dumas, P. and Sultan 13

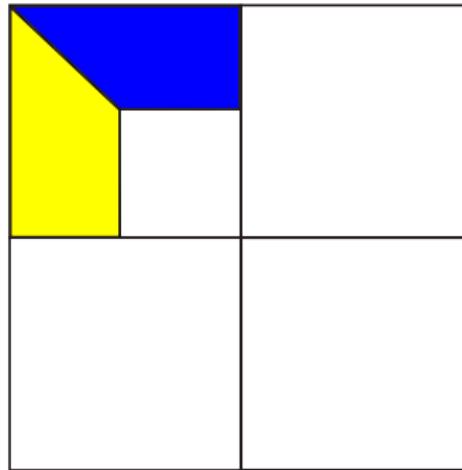


2×2 block splitting

The tiled recursive algorithm



Dumas, P. and Sultan 13

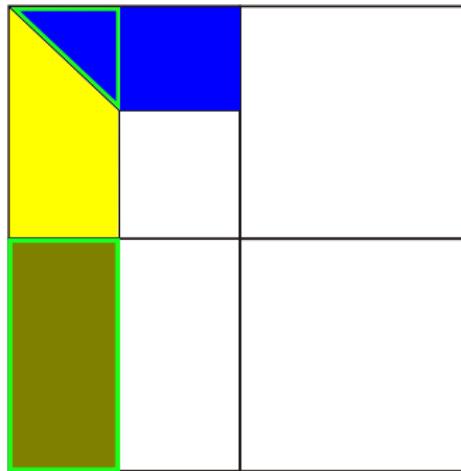


Recursive call

The tiled recursive algorithm



Dumas, P. and Sultan 13

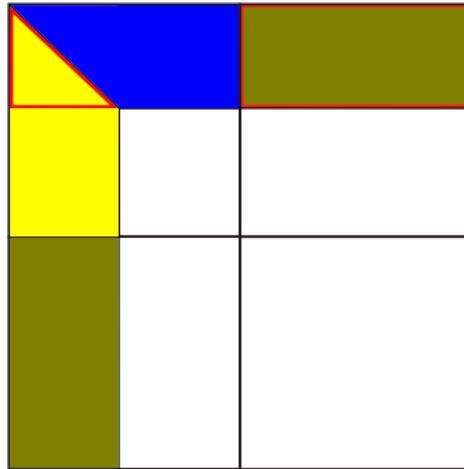


TRSM: $B \leftarrow BU^{-1}$

The tiled recursive algorithm



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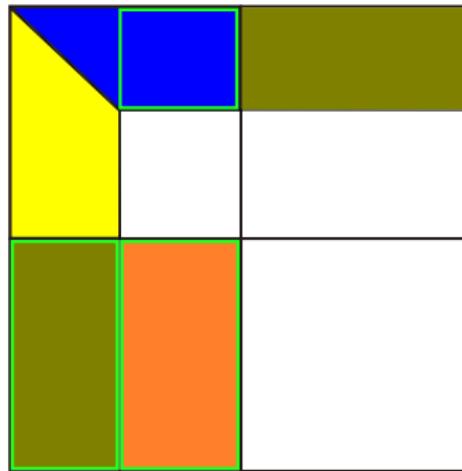


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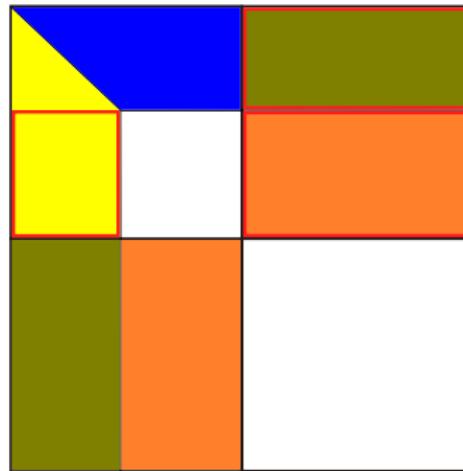


MatMul: $C \leftarrow C - A \times B$

The tiled recursive algorithm



Dumas, P. and Sultan 13

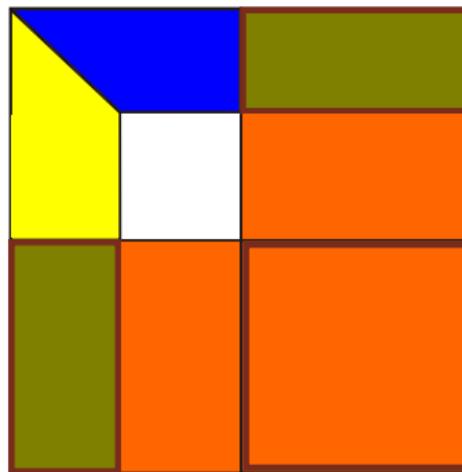


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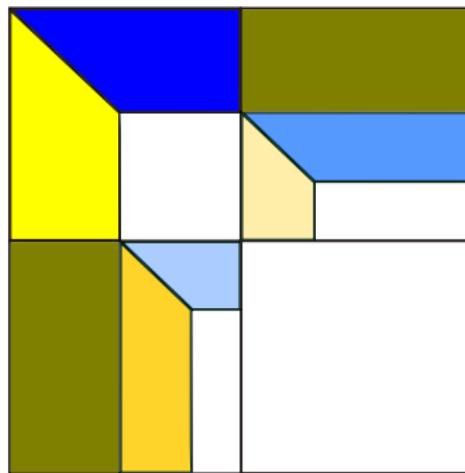


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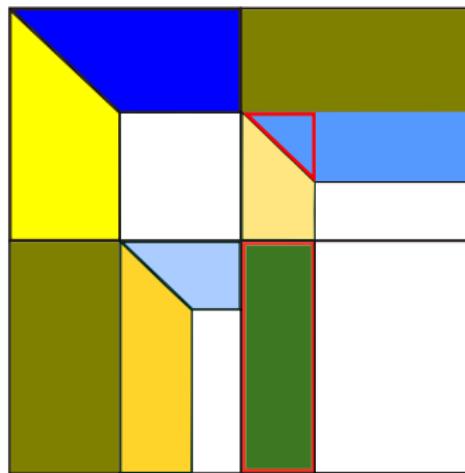


2 independent recursive calls (compatible with the **product order**)

The tiled recursive algorithm



Dumas, P. and Sultan 13

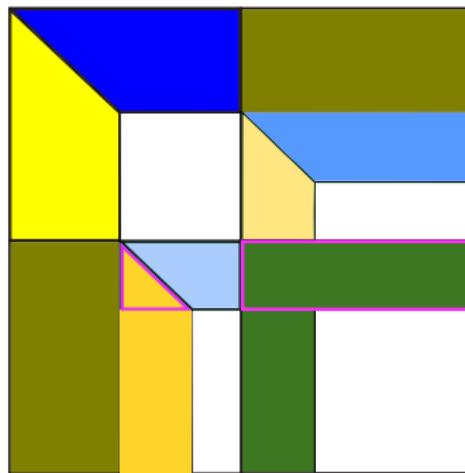


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The tiled recursive algorithm



Dumas, P. and Sultan 13

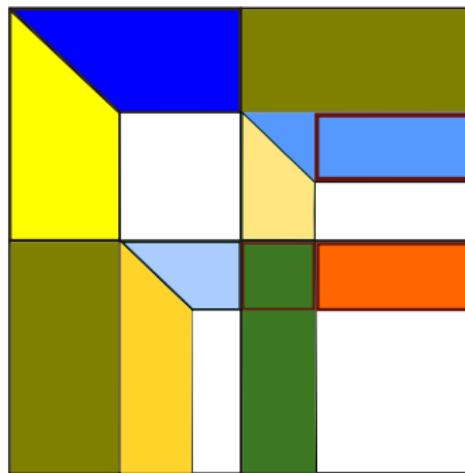


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The tiled recursive algorithm



Dumas, P. and Sultan 13

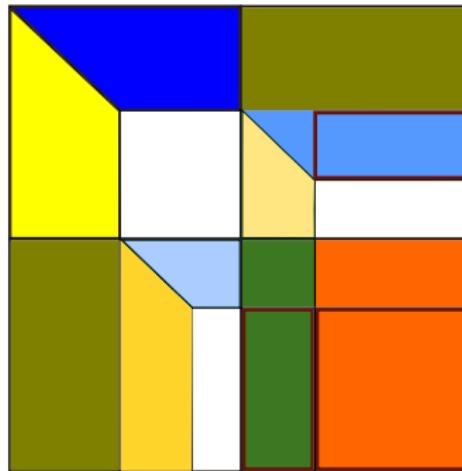


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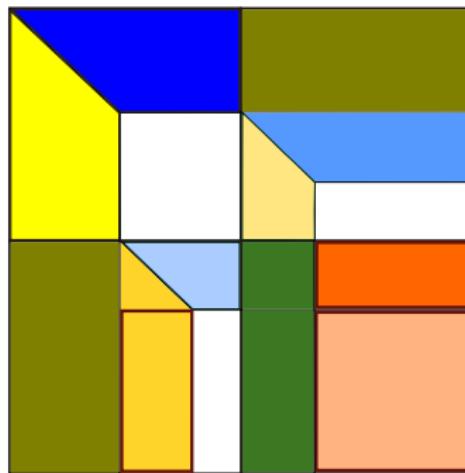


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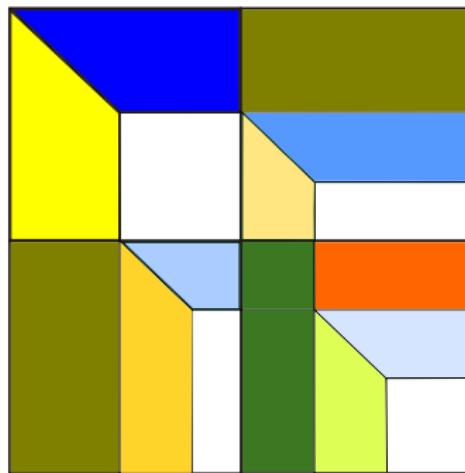


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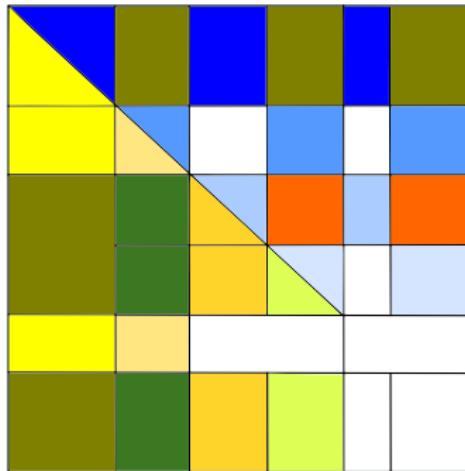


Recursive call

The tiled recursive algorithm



Dumas, P. and Sultan 13

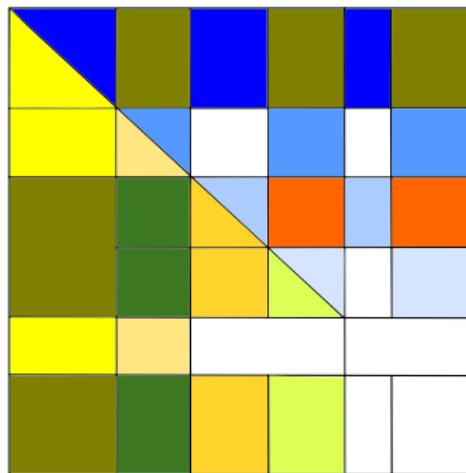


Puzzle game (block **rotations**)

The tiled recursive algorithm



Dumas, P. and Sultan 13



- ▶ $O(mnr^{\omega-2})$ ($2/3n^3$ for $\omega = 3$)
- ▶ fewer modular reductions than slab algorithms
- ▶ rank deficiency introduces parallelism

Iterative algorithms

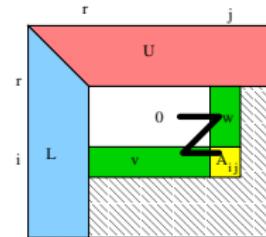
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Iterative algorithms

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Which base case algorithm?

- ▶ Formerly [DPS13]: **product order** iterative algorithm
 - ✗ many permutations
 - ✗ many modular reductions

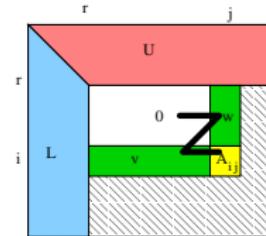


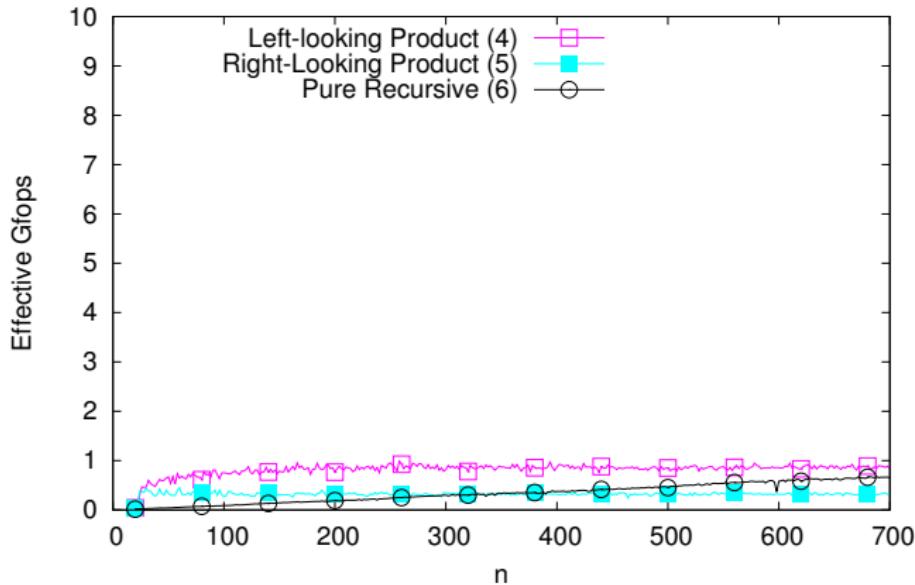
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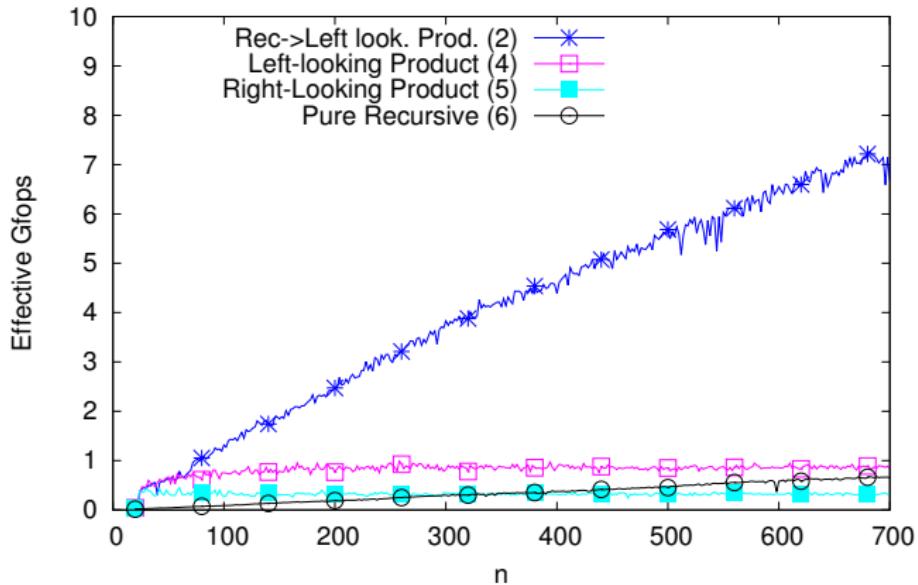
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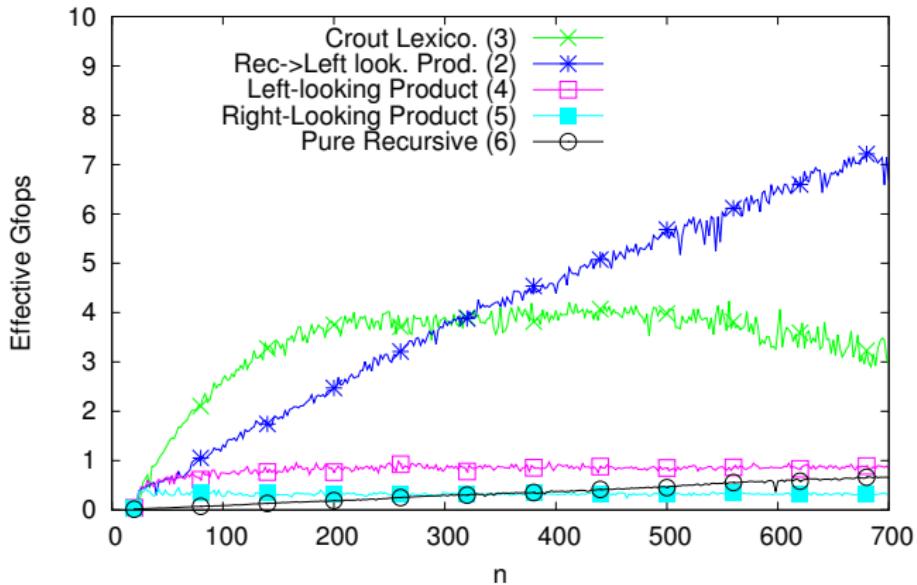
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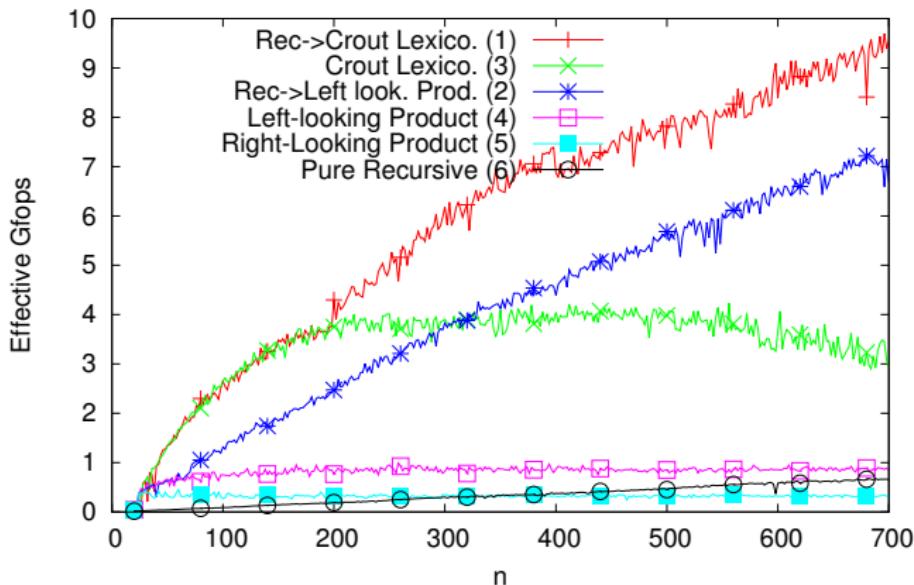
- ▶ Formerly [DPS13]: **product order** iterative algorithm
 - \times many permutations
 - \times many modular reductions
- ▶ [DPS15]: Simply use the schoolbook algorithm (Lexico+Rotations)
 - \checkmark fewer permutations
 - \checkmark modular reductions delayed more easily
 - \checkmark Crout variant: better data access pattern

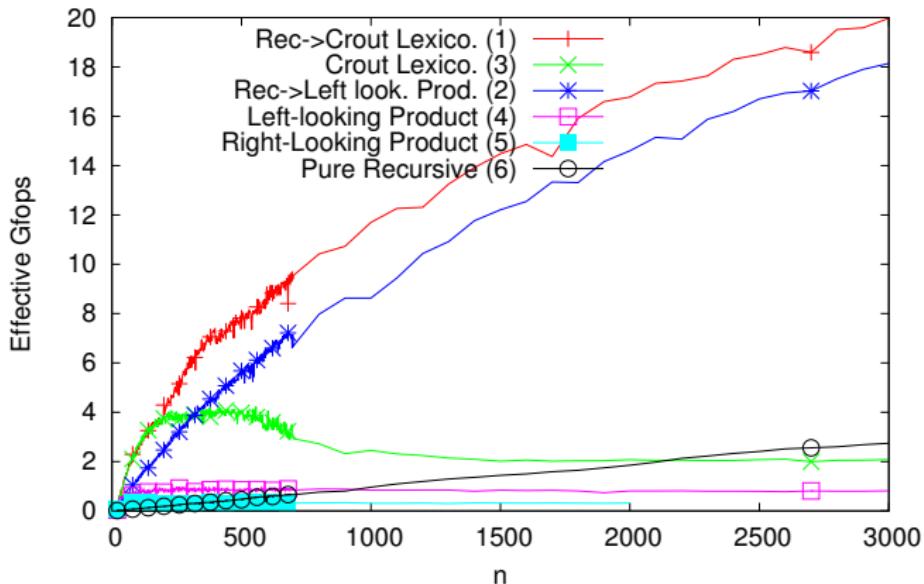


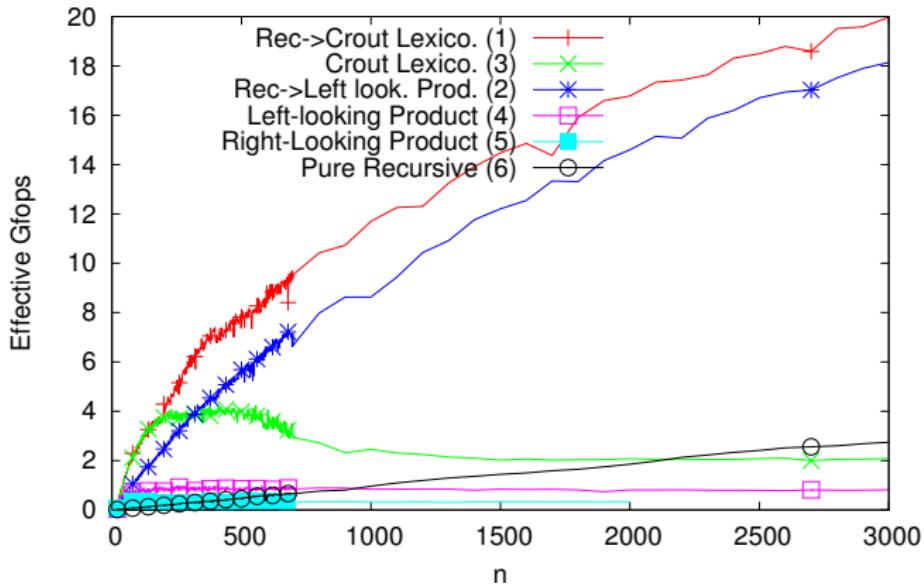
PLUQ base cases mod 131071. Rank = $n/2$. on a i5-3320 at 2.6GHz

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- ▶ > 2 Gflops improvement
- ▶ Implemented in FFLAS-FFPACK (kernel of LinBox).

Outline

- 1 The rank profile Matrix
- 2 Computing the rank profile matrix
- 3 Algorithmic instances
- 4 Relations to other decompositions
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Malaschonok LEU decomposition

[Malaschonok'10]: $A = L \cdot E \cdot U$

- ▶ E is an r -sub-permutation matrix
- ▶ Designed to avoid permutations
- ▶ $\frac{17}{2^\omega - 4} MM(m, n)$ with $m = n = 2^k$.
- ▶ no connection to rank profile nor echelon form
- ▶ no rank sensitive complexity

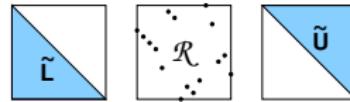
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Fact

$$E = \mathcal{R}^A$$



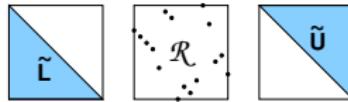
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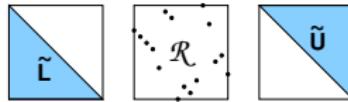
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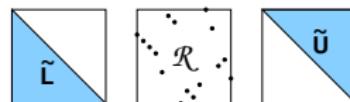
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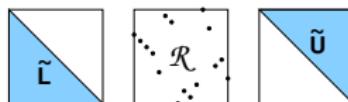
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With appropriate pivoting:

$$\Pi_{P,Q} = \mathcal{R}(A)$$

LUP and PLU decompositions

LUP

If A has generic RowRP

- ▶ $LUP(A)$ with Lex order and col. rot.: $\rightsquigarrow \begin{bmatrix} I_r & \\ & 0 \end{bmatrix} P = \mathcal{R}^A$

In particular, if A has full row rank and $m = n$:

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PLU

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In particular, if A has full column rank and $m = n$: $\rightsquigarrow P = \mathcal{R}^A$

Bruhat decomposition

- ▶ If $A = \tilde{L}\mathcal{R}^A\tilde{U}$, then
 - ▷ For J_n the unit anti-diagonal matrix,
 - ▷ $V = J_n\tilde{L}J_n$ is upper triangular
 - ▷ $\tilde{\mathcal{R}} = J_n\mathcal{R}^A$ is a rank r sub-permutation
 - ▷ $A = V\tilde{\mathcal{R}}\tilde{U}$ (Bruhat decomposition)

$$V$$

$$\tilde{\mathcal{R}}$$

$$\tilde{U}$$

Echelon forms

$$\mathcal{R}_A = P \cdot Q$$

for

$$P \quad L \quad U \quad Q$$

$$C = PLP_s$$

sort

$$Q_s U Q = E$$

Outline

- 1 The rank profile Matrix
- 2 Computing the rank profile matrix
- 3 Algorithmic instances
- 4 Relations to other decompositions
- 5 Generalization over a Ring
- 6 The small rank case

The rank profile matrix over a Ring R

Notion of rank over a Ring

Spanning rank:

$$s_R(A) = \min\{r : A = BC \text{ where } B \text{ is } m \times r \text{ and } C \text{ is } r \times n\}.$$

McCoy's rank:

- ▶ $\mathcal{M}_R(A) = \max$ size of a non zero minor in A
- ▶ largest number of cols of A with right nullspace $= \{0\}$

Smith's rank: (over a PIR) $\mathcal{S}_R = \text{number of unit Smith invariants} = \mathcal{M}_R$

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Over a Principal Ideal Domain

Define K_R , the field of fractions of R . \rightsquigarrow notion of field rank r_{K_R} .

Fact: $s_R = \mathcal{M}_R = r_{K_R}$.

\rightsquigarrow same rank profile matrix

The rank profile matrix over a Ring with zero divisors

Example

Over $\mathbb{Z}/4\mathbb{Z}$, consider $A = \begin{bmatrix} 0 & 2 \\ 2 & 1 \end{bmatrix}$

- ▶ $s_R(A) = 1$ as $A = \begin{bmatrix} 2 \\ 1 \end{bmatrix} [2 \ 1]$
- ▶ Then $\mathcal{R}^A = \begin{bmatrix} 0 & b \\ c & d \end{bmatrix}$ with $b, c \neq 0$.
- ▶ But $d \neq 0$ as $\begin{bmatrix} 0 & b \\ c & d \end{bmatrix} = \begin{bmatrix} x \\ y \end{bmatrix} [z \ t] \Rightarrow x, y, z, t \neq 0 \Rightarrow \begin{cases} x = z = 2, \\ y, t = -1 \end{cases}$

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But $\mathcal{M}_R([0 \ 2]) = 0$, hence $\mathcal{R}(A) = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$ with McCoy's rank.

The rank profile matrix over a Ring

Theorem

Over an arbitrary ring, the Rank profile matrix can always be defined using McCoy's rank.

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Small rank

When $r \ll m, n$, $O(mnr^{\omega-2})$ can be too expensive.
(Compressed sensing applications)

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Can the rank profile matrix be computed in such complexities?

[Storjohann Yang'14] Linear System Oracle

Sketch of the $O(r^3 + mn)$ algorithm

Incrementally for $s = 1.. \text{rank}(A)$, maintain

- ▶ an $s \times s$ invertible sub-matrix A_s of A .
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$\rightsquigarrow O(sn)$

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Lexico. search with rotations \rightsquigarrow computes \mathcal{R}^A

[Storjohann Yang'15] Relaxed matrix inverse

Sketch of the algorithm: RowRP in $\tilde{O}(r^\omega + mn)$

- ① Instead of building A_s^{-1} iteratively ($O(r^3)$), use an asymptotically fast relaxation scheme $O(r^\omega)$.
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Perspective

- ▶ Application to F5 elimination (Gröbner basis) [Sun Lin Wang'14]
- ▶ Communication avoiding variants [Demmel & Al.'12]
- ▶ How to accomodate sparse elimination constraints ?
- ▶ Numerical pivoting equivalent?

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Thank you!

Bibliography

[Malaschonok'10]: $A = LEU$

- ▶ first instance of \mathcal{R}^A .
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[DSP'13]: $A = PLUQ$

Computed only via a product order pivoting,
Rank sensitive $O(r^{\omega-2}mn)$, any $m \times n$ matrix of any rank r .

[DPS'15]

- ▶ Conditions for any PLUQ alg. to reveal \mathcal{R}^A
- ▶ New pivoting strategies \rightsquigarrow faster base case

[DPS'XX in preparation]

- ▶ \mathcal{R}^A in $O(r^\omega + mn)$
- ▶ generalization of \mathcal{R}^A to rings