Fast exact linear algebra: LinBox

Clément Pernet

SAGE Days 6,
November 11, 2007

Outline

LinBox: an overview
- Principles
- Organisation of the library
- Dense computations
- BlackBox computations

Memory efficient implementations
- In-place eliminations
- Fast matrix multiplication

Linear algebra over big integers

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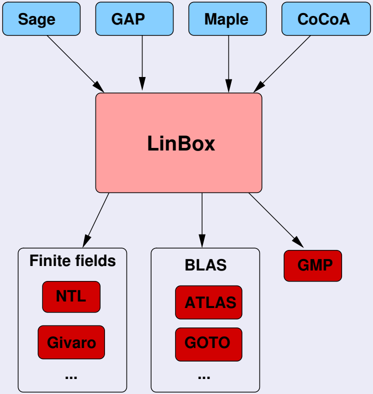
LinBox

A generic middleware



The LinBox project, facts

Joint NSF–CNRS project.

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A LGPL source library:

- 122 000 lines of C++ code
- 5-10 active developers

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2008	Towards a major change of interface (simpler) v2.0

LinBox-1.0

Solutions

- rank
- det
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Matrices

- Sparse, structured
- Dense

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A design for genericity

Field/Ring interface

- Shared interface with Givaro
- Wraps NTL, Givaro implementations, using archetype or envelopes
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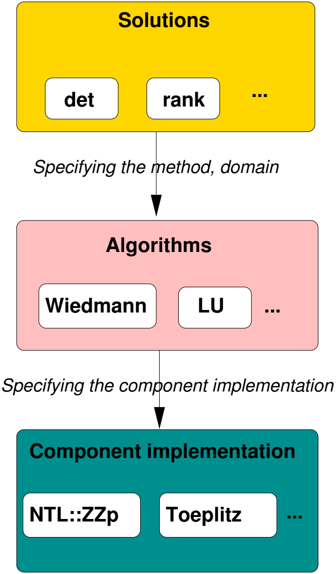
Matrix interface

- Sparse, Structured, Dense: BlackBox `apply`
- Dense matrix interface: several levels of abstraction

Structure of the library



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NTL::ZZp F(65521);
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Dense computations: FFLAS−FFPACK

Building block:

matrix multiplication over word-size finite field

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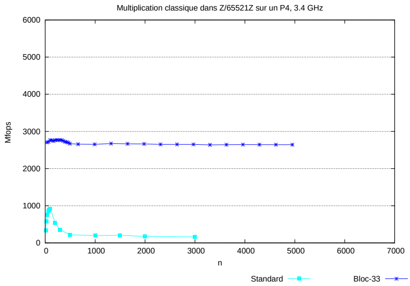
$\Rightarrow$ rely on the existing BLAS



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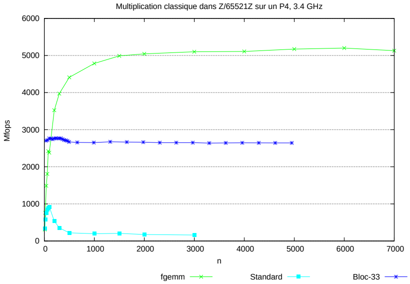

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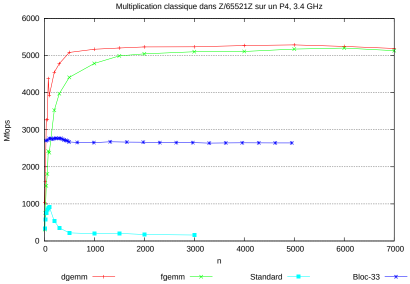

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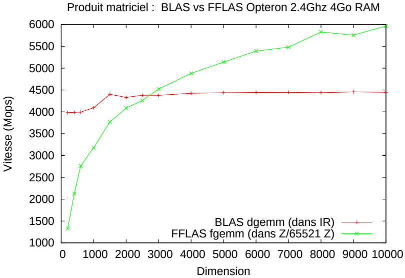
- Sub-cubic algorithm (Winograd)



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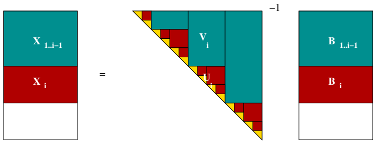

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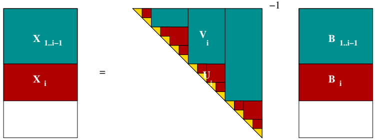

	n	1000	2000	3000	5000	10 000
TRSM	$\frac{ftrsm}{dtrsm}$	1,66	1,33	1,24	1,12	1,01
LQUP	$\frac{lqup}{dgetrf}$	2,00	1,56	1,43	1,18	1,07
INVERSE	$\frac{inverse}{dgetrf+dgetri}$	1.62	1.32	1.15	0.86	0.76

Characteristic polynomial

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- Frobenius normal form as well
- Transformation in $\mathcal{O}(n^\omega \log\log n)$

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BlackBox computations

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Goal: computation with very large sparse or structured matrices.

- No explicit representation of the matrix,
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- No explicit representation of the matrix,
- Only operation: application of a vector
- Efficient algorithms
- Efficient preconditionners: Toeplitz, Hankel, Butterfly, ...

Block projection algorithms

- Wiedemann algorithm: scalar projections of A^i for $i = 1..2d$
- Block Wiedemann: $k \times k$ dense projections of A^i for $i = 1..2d/k$

$\Rightarrow$Balance efficiency between BlackBox and dense compations

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Memory efficient dense linear algebra

Structure of dense algorithms: reduction to `matmul`

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Approach:

1. Memory efficient reductions to `matmul` (ideally in-place)
2. Reduce extra memory requirements for `matmul`

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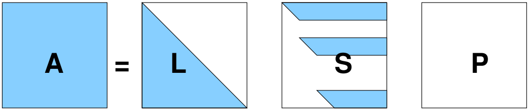
  Ibarra, Moran, Hui 82 : $A = LSP$, in $\mathcal{O}\left(n^\omega\right)$
  Ibarra, Moran, Hui 82 : $A = LQUP$, in $\mathcal{O}\left(n^\omega\right)$

LSP-LQUP decompositions



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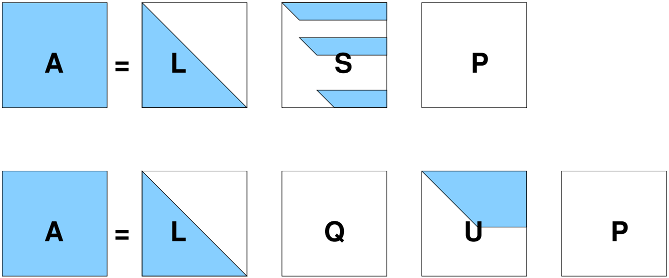

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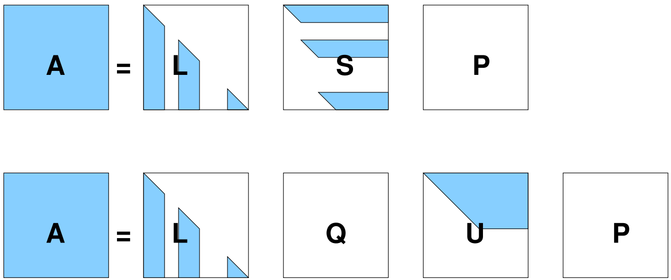
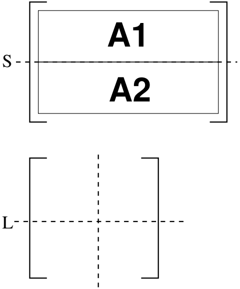


The LSP algorithm



1. Split A Row-wise

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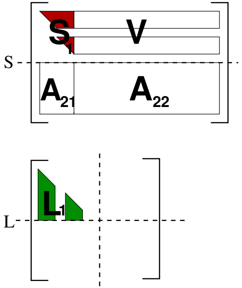

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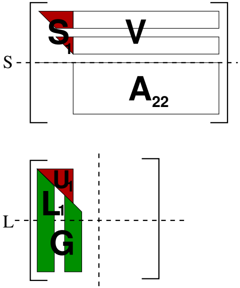

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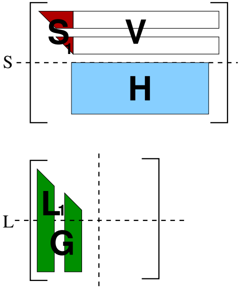

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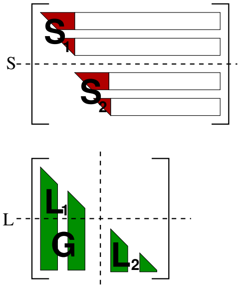

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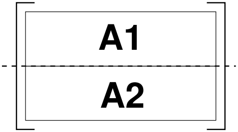
The LQUP decomposition



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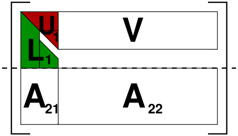

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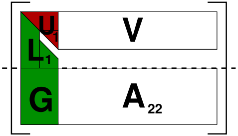

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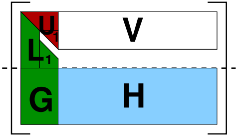

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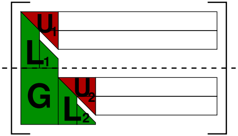

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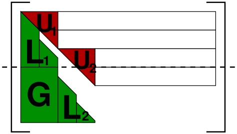

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6. Row permutations

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Choice of the LQUP decomposition as a building block:

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Choice of the LQUP decomposition as a building block:

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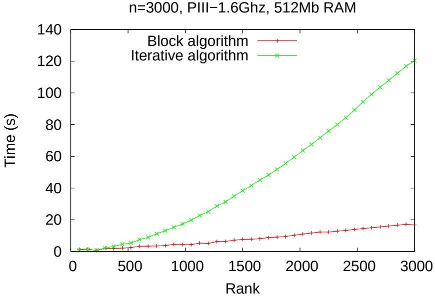
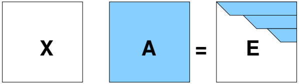
- in-place computation
- Permutation Q describes the row rank profile of A
- Rank sensitive computation time: $\mathcal{O}\left(mnr^{\omega-2}\right)$



Echelon forms

Row Echelon Form $XA = E$



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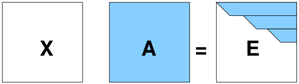
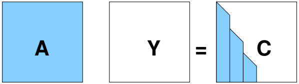


Column Echelon Form $AY = C$



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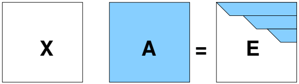

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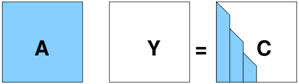

Property (Link with LQUP)

$$C = LQ \begin{bmatrix} I_r \\ 0 \end{bmatrix}, \qquad Y = P^T \begin{bmatrix} U_1 & U_2 \\ 0 & I_{n-r} \end{bmatrix}^{-1}$$

From LQUP to Column Echelon

Additional operations:

- $-U^{-1}U_2$ `trsm` (triangular system solve) in-place

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TRTRI: triangular inverse

$$\begin{bmatrix} U_1 & U_2 \\ & U_3 \end{bmatrix}^{-1} = \begin{bmatrix} U_1^{-1} & -U_1^{-1}U_2U_3^{-1} \\ & U_3^{-1} \end{bmatrix}$$

1: **if** $n = 1$ **then**
2: $\quad U \leftarrow U^{-1}$
3: **else**
4: $\quad U_2 \leftarrow U_3^{-1}U_2$ TRSM
5: $\quad U_2 \leftarrow -U_2U_3^{-1}$ TRSM
6: $\quad U_1 \leftarrow U_1^{-1}$ TRTRI
7: $\quad U_3 \leftarrow U_3^{-1}$ TRTRI
8: **end if**

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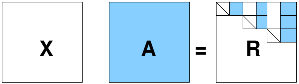

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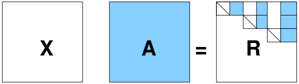
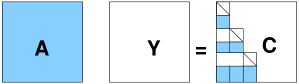


Column Reduced Echelon Form $AY = C$



From Echelon to Reduced Echelon

Again reduces to:

$U^{-1}X$: `TRSM`, in-place

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`TRTRM`: triangular triangular multiplication

$$\begin{bmatrix} U_1 & U_2 \\ & U_3 \end{bmatrix} \begin{bmatrix} L_1 & \\ L_2 & L_3 \end{bmatrix} = \begin{bmatrix} U_1L_1 + U_2L_2 & U_2L_3 \\ U_3L_2 & U_3L_3 \end{bmatrix}$$

1: $X_1 \leftarrow U_1L_1$ `TRTRM`
2: $X_1 \leftarrow X1 + U_2L_2$ `MM`
3: $X_2 \leftarrow U_2L_3$ `TRMM`
4: $X_3 \leftarrow U_3L_2$ `TRMM`
5: $X_4 \leftarrow U_3L_3$ `TRTRM`

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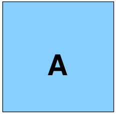
Example

A has full rank and generic rank profile.



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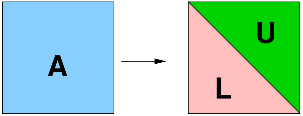
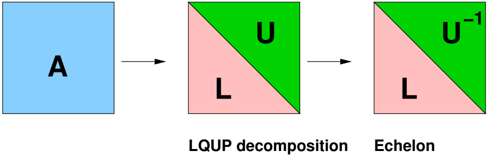


LQUP decomposition

$$A = LU$$

Example

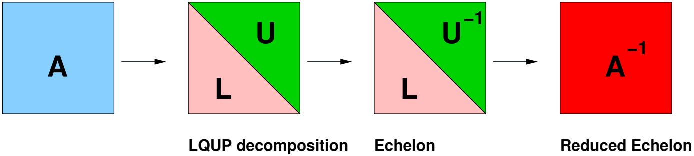
A has full rank and generic rank profile.



$$AU^{-1} = L$$

Example

A has full rank and generic rank profile.



$$A(U^{-1}L^{-1}) = I$$

Summary

Global scheme of reductions to LQUP decomposition.
Ensures:

- in-place computations

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Global scheme of reductions to LQUP decomposition.
Ensures:

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- increases modularity

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These reductions are "efficient" with regard to the constant C_3 where $\mathcal{O}(n^3) = C_3 n^3$:

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cost	$2/3$	$2/3$	$2/3$	1	2

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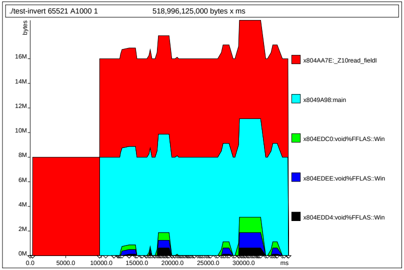
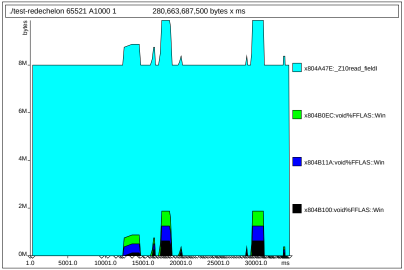
Experiments





Outline

Strassen-Winograd algorithm

$$\begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix},$$

- 8 additions:

$$\begin{array}{ll} S_1 \leftarrow A_{21} + A_{22} & T_1 \leftarrow B_{12} - B_{11} \\ S_2 \leftarrow S_1 - A_{11} & T_2 \leftarrow B_{22} - T_1 \\ S_3 \leftarrow A_{11} - A_{21} & T_3 \leftarrow B_{22} - B_{12} \\ S_4 \leftarrow A_{12} - S_2 & T_4 \leftarrow T_2 - B_{21} \end{array}$$

- 7 recursive multiplications:

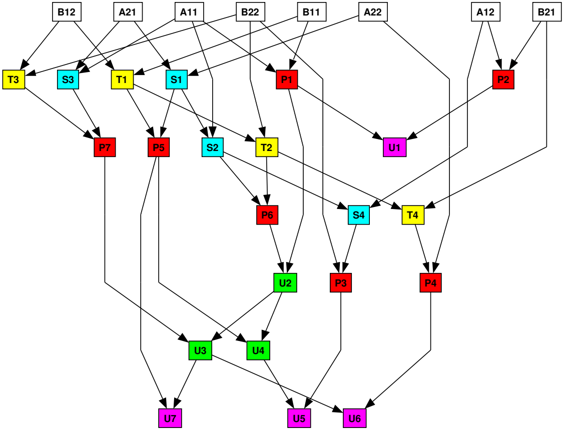
$$\begin{array}{ll} P_1 \leftarrow A_{11} \times B_{11} & P_5 \leftarrow S_1 \times T_1 \\ P_2 \leftarrow A_{12} \times B_{21} & P_6 \leftarrow S_2 \times T_2 \\ P_3 \leftarrow S_4 \times B_{22} & P_7 \leftarrow S_3 \times T_3 \\ P_4 \leftarrow A_{22} \times T_4 & \end{array}$$

- 7 final additions:

$$\begin{array}{ll} U_1 \leftarrow P_1 + P_2 & U_5 \leftarrow U_4 + P_3 \\ U_2 \leftarrow P_1 + P_6 & U_6 \leftarrow U_3 - P_4 \\ U_3 \leftarrow U_2 + P_7 & U_7 \leftarrow U_3 + P_5 \\ U_4 \leftarrow U_2 + P_5 & \end{array}$$

- The result is the matrix: $C = \begin{bmatrix} U1 & U5 \\ U6 & U7 \end{bmatrix}$

Tasks dependencies



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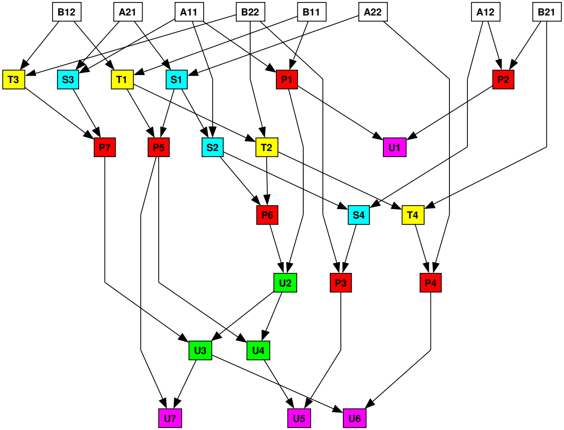

- Extra temporary blocks required
- Pebble game to minimize their number [Huss-Ledermann & Al. 96]

Reducing memory requirements

Dealing with 2 kind of computations:

- $C \leftarrow A \times B$
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Previous work: [Huss-Ledermann & Al. 96].

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- Inputs can be overwritten — $Cn^{2.8} + \epsilon n^{2.8}$
- Add a few pre-additions — $Cn^{2.8} + \epsilon n^{2.8}$
- Cascading with classical algorithm — $Cn^{2.8} + \epsilon n^{2.8}$

Results

Adding pre-additions:

#	operation	loc.	#ř	operation	loc.
1	$C_{22} = C_{22} - C_{12}$	C_{22}	13	$P_3 = S_4 B_{22} + C_{12}$	C_{12}
2	$C_{21} = C_{21} - C_{22}$	C_{21}	14	$P_1 = A_{11} B_{11}$	X_1
3	$C_{12} = C_{12} - C_{22}$	C_{12}	15	$U_2 = P_6 + P1$	C_{21}
4	$S_1 = A_{21} + A_{22}$	X_1	16	$P_2 = A_{12} B_{21} + C_{11}$	C_{11}
5	$T_1 = B_{12} - B_{11}$	X_2	17	$U_1 = P_1 + P_2$	C_{11}
6	$P_5 = S_1 T_1 + C_{12}$	C_{12}	18	$U_5 = U_2 + C_{12}$	C_{12}
7	$S_2 = S_1 - A_{11}$	X_1	19	$S_3 = A_{11} - A_{21}$	X_1
8	$T_2 = B_{22} - T_1$	X_2	20	$T_3 = B_{22} - B_{12}$	X_2
9	$P_6 = S_2 T_2 + C_{21}$	C_{21}	21	$U_3 = P_7 + U_2 = S_3 T_3 + U_2$	C_{21}
10	$S_4 = A_{12} - S_2$	X_1	22	$U_7 = U_3 + C_{22}$	C_{22}
11	$T_4 = T_2 - B_{21}$	X_2	23	$U_6 = U_3 - P_4 = -A_{12} T_4 + U_3$	C_{21}
12	$C_{22} = P_5 + C_{22}$	C_{22}			

- $C \leftarrow A \times B + C$ $\Rightarrow$ from 3 to 2 temp. (3 pre-adds)

Results

Overwriting inputs:

#	operation	loc.	#ř	operation	loc.
1	$C_{21} = C_{21} - C_{22}$	C_{21}	13	$P_4 = A_{22}T_4 + \beta C_{21}$	C_{21}
2	$C_{22} = C_{22} - C_{12}$	C_{22}	14	$P_2 = A_{12}B_{21} + \beta C_{11}$	C_{11}
3	$S_3 = A_{11} - A_{21}$	X	15	$P_1 = A_{11}B_{11}$	B_{21}
4	$T_3 = B_{22} - B_{12}$	Y	16	$U_1 = P_1 + P_2$	C_{11}
5	$P_7 = S_3T_3 + \beta C_{22}$	C_{22}	17	$P_6 = S_2T_2$	A_{12}
6	$S_1 = A_{21} + A_{22}$	A_{21}	18	$U_2 = P_1 + P_6$	C_{12}
7	$T_1 = B_{12} - B_{11}$	B_{12}	19	$U_4 = U_2 + P_5$	C_{12}
8	$S_2 = S_1 - A_{11}$	X	20	$U_3 = U_2 + P_7$	C_{22}
9	$T_2 = B_{22} - T_1$	Y	21	$U_7 = U_3 + P_5$	C_{22}
10	$P_5 = S_1T_1 + \beta C_{12}$	C_{12}	22	$U_6 = U_3 - P_4$	C_{21}
11	$S_4 = A_{12} - S_2$	A_{21}	23	$P_3 = S_4B_{22}$	A_{12}
12	$T_4 = T_2 - B_{21}$	B_{12}	24	$U_5 = U_4 + P_3$	C_{12}

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Results

Overwriting inputs:

#	operation	loc.	#ř	operation	loc.
1	$S_3 = A_{11} - A_{21}$	C_{11}	12	$S_4 = A_{12} - S_2$	C_{22}
2	$S_1 = A_{21} + A_{22}$	A_{21}	13	$P_6 = S_2 T_2$	C_{12}
3	$T_1 = B_{12} - B_{11}$	C_{22}	14	$U_2 = P_1 + P_6$	C_{12}
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- $C \leftarrow A \times B$ $\Rightarrow$fully in-place

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Question:

Is there an in-place $\mathcal{O}\left(n^{2.807}\right)$ algorithm with constant inputs?

Results

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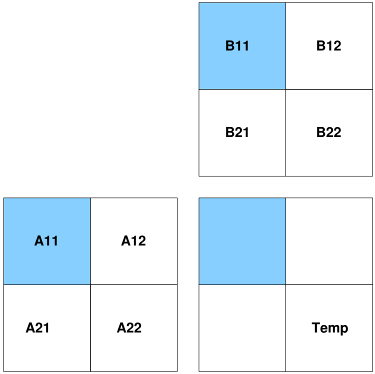
$\Rightarrow$yes

Principle of the fully in-place algorithm



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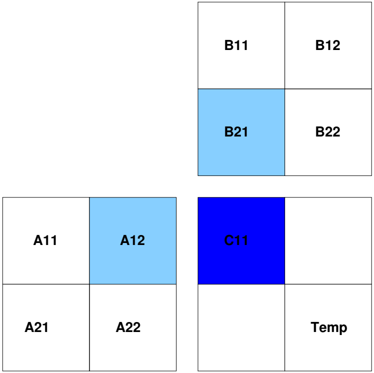

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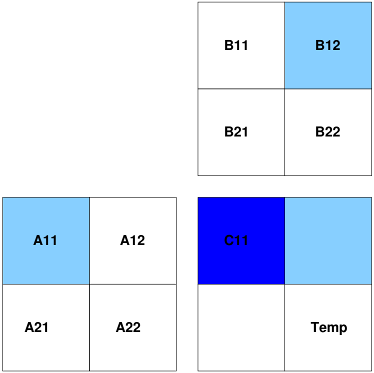

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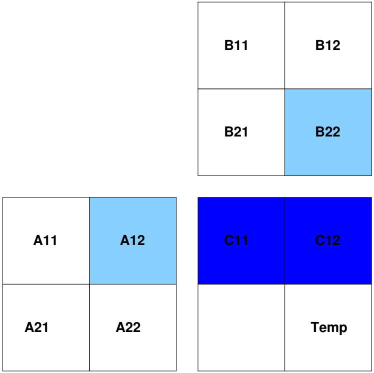

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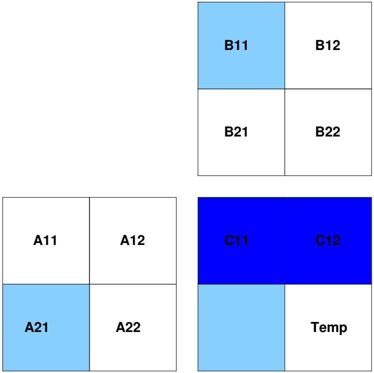

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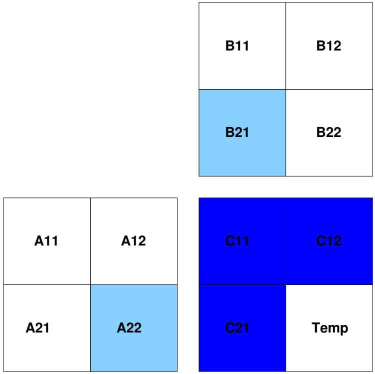

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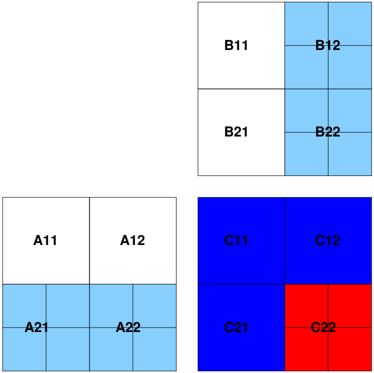

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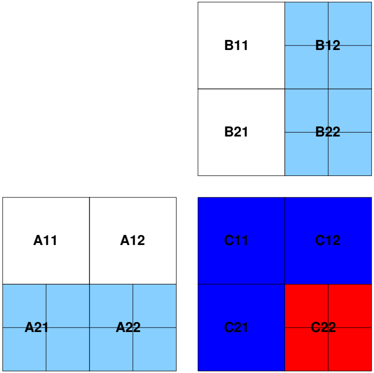

- $7.2n^{2.807}$ instead of $6n^{2.807}$

Outline

LinBox: an overview

- Principles
- Organisation of the library
- Dense computations
- BlackBox computations

Memory efficient implementations

- In-place eliminations
- Fast matrix multiplication

Linear algebra over big integers

The problem

- Reasonably small dimension ($n = 2..100$)
- Unreasonably large entries
  ($\log_2 \|A\|_\infty = 1,000,000..1,000,000,000$)

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The problem

- Reasonably small dimension ($n = 2..100$)
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$$\texttt{mul} \gg \texttt{add}$$

despite FFT

- Fast Matrix Multiplication is always better than classic,
- Can do better than Strassen-Winograd

Dealing with odd dimensions

Padding: add 0 columns and rows to the nearest power of 2 (more operations)

Peeling: slice down to the nearest power of 2, and use classical block algorithm (less “sub-cubic”).

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Dealing with odd dimensions

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Static: Before actual computation.

Dynamic: At each recursive level, dimension 1 modifications.

Virtual dynamic padding:

- Recursive splitting with odd dimensions
- No extra operations (virtual 0)
- Better operation count than peeling

Winograd 68

Formula for dot-product:

$$a_1 b_1 + a_2 b_2 = (a_1 + b_2)(a_2 + b_1) - a_1 a_2 - b_1 b_2$$

Winograd 68

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$$a_1 b_1 + a_2 b_2 = (a_1 + b_2)(a_2 + b_1) - a_1 a_2 - b_1 b_2$$

for k=1..n/2 **do**
  for i=1..n **do**
    $\alpha_{i,k} = (a_{i,2k} a_{i,2k+1})$
  end for
  for j=1..n **do**
    $\beta_{k,j} = (b_{2k,j} b_{2k+1,j})$
  end for
  for i=1..n **do**
    for j=1..n **do**
      $C_{i,j} += (a_{i,2k} + b_{2k+1,j})(a_{i,2k+1} + b_{2k,j}) - \alpha_{i,k} - \beta_{k,j}$
    end for
  end for
end for

Winograd 68

Formula for dot-product:

$$a_1 b_1 + a_2 b_2 = (a_1 + b_2)(a_2 + b_1) - a_1 a_2 - b_1 b_2$$

for k=1..n/2 **do**
    for i=1..n **do**
        $\alpha_{i,k} = (a_{i,2k} a_{i,2k+1})$
    end for
    for j=1..n **do**
        $\beta_{k,j} = (b_{2k,j} b_{2k+1,j})$
    end for
    for i=1..n **do**
        for j=1..n **do**
            $C_{i,j} += (a_{i,2k} + b_{2k+1,j})(a_{i,2k+1} + b_{2k,j}) - \alpha_{i,k} - \beta_{k,j}$
        end for
    end for
end for

- Requires commutativity (no recursive algorithm)
- Still $\mathcal{O}(n^3)$
- But better constant: $T_2(n) = 1/2n^3 + n^2$ instead of $1n^3$

From 2 to 3

$$a_1 b_1 + a_2 b_2 + a_3 b_3 = (a_1 + a_2 + b_3)(a_3 + b_1 + b_2)$$

$$T_3(n) = 1/3n^3$$

From 2 to 3

$$a_1b_1 + a_2b_2 + a_3b_3 = (a_1 + a_2 + b_3)(a_3 + b_1 + b_2) - (a_1 + a_2)a_3 - b_3(b_1 + b_2)$$

$$T_3(n) = 1/3n^3 \qquad + 2/3n^2$$

From 2 to 3

$$\begin{aligned} a_1 b_1 + a_2 b_2 + a_3 b_3 &= (a_1 + a_2 + b_3)(a_3 + b_1 + b_2) \\ &\quad - (a_1 + a_2) a_3 - b_3 (b_1 + b_2) \\ &\quad - a_1 b_2 - a_2 b_1 \end{aligned}$$

$$T_3(n) = 1/3 n^3 + T(n, 2/3 n) + 2/3 n^2$$

Comparison

n	2	3	4	6	8
Classical algorithm	8	27	64	216	512
Strassen+Peeling	**7**	26	49	182	343

n	9	10	12	15	18
Classical algorithm	729	1000	1728	3375	5832
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New algorithm	**489**		1088	**2093**	3456

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- ...including rectangular matrices,
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- automatically generate a combination of base case algorithms for a given dimension