High-performance matrix computations: It's not all about libraries

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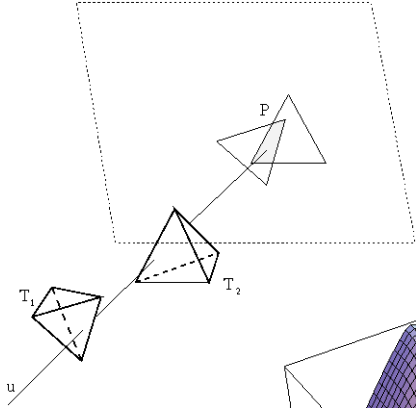
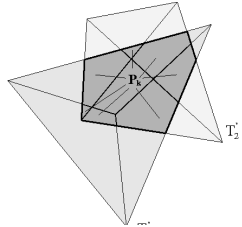
About me

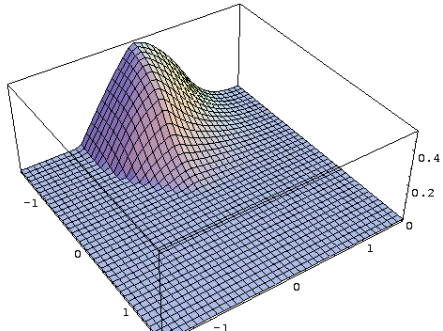
Italy – Tuscany

Italy – University of Pisa

Computational Geometry







USA – UT Austin, TX

- Symmetric eigenproblem
  $\boldsymbol{AX = X\Lambda}$
- FLAME project
  Automatic generation of algorithms

Algorithm $LU = A$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right), L \rightarrow \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array}\right), U \rightarrow \left(\begin{array}{c|c} U_{TL} & U_{TR} \\ \hline 0 & U_{BR} \end{array}\right)$

where $A_{TL}, L_{TL}, U_{TL},$ are 0×0

While $m(A_{TL}) \leq m(A)$ **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right), \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} L_{00} & 0 & 0 \\ \hline l_{10}^T & 1 & 0 \\ \hline L_{20} & l_{21} & L_{22} \end{array}\right),$$

$$\left(\begin{array}{c|c} U_{TL} & U_{TR} \\ \hline 0 & U_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} U_{00} & u_{01} & U_{02} \\ \hline 0 & \upsilon_{11} & u_{12}^T \\ \hline 0 & 0 & U_{22} \end{array}\right)$$

where $\alpha_{11}, 1, \upsilon_{11}$ are scalars

$$\upsilon_{11} := \alpha_{11} - l_{10}^T u_{01}$$
$$u_{12}^T := a_{12}^T - l_{10}^T U_{02}$$
$$l_{21} := (a_{21} - L_{20} u_{01}) / \upsilon_{11}$$

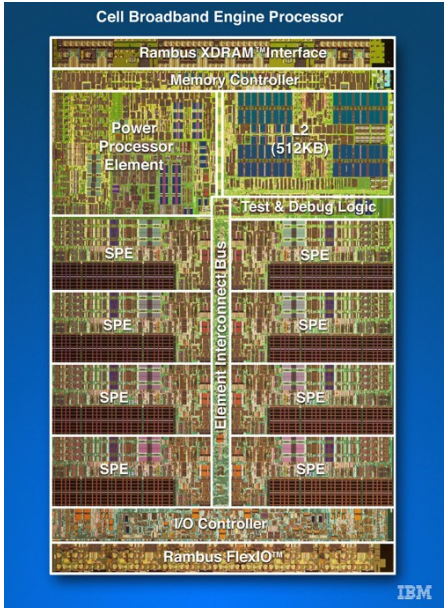
Continue with

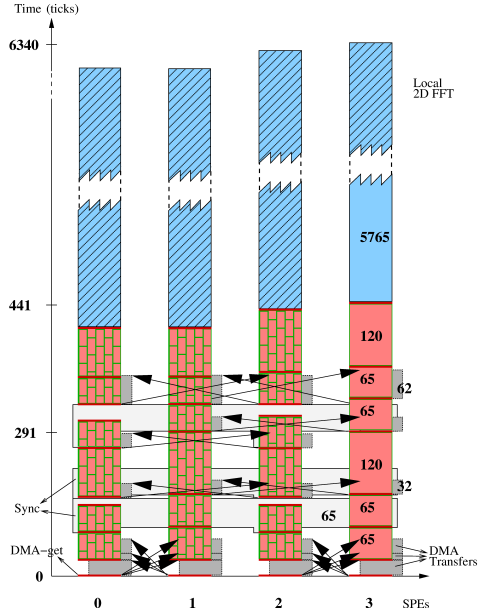
$$\left(\begin{array}{c|c} A_{TL} & A_{TR} \\ \hline A_{BL} & A_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & a_{01} & A_{02} \\ \hline a_{10}^T & \alpha_{11} & a_{12}^T \\ \hline A_{20} & a_{21} & A_{22} \end{array}\right), \left(\begin{array}{c|c} L_{TL} & 0 \\ \hline L_{BL} & L_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} L_{00} & 0 & 0 \\ \hline l_{10}^T & 1 & 0 \\ \hline L_{20} & l_{21} & L_{22} \end{array}\right), \cdots$$

endwhile

USA – Duke, NC

- Cell
- FFTs





Germany – RWTH Aachen University

High-Performance &
Automatic Computing

Modern
Inverse
Problems

Sweden – Umeå University

- Matrix & tensor operations
- HPC
- Computer music

HPC2N

High-Performance Computing Center North

Outline

- Part 1: Short intro
- Part 2: Numerical linear algebra: historical overview
- Part 3: Linear Algebra Mapping Problem (LAMP)
  Use and misuse of libraries

30-second lecture

30-second lecture

- Computers are great with numbers (scalars)

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- Domain experts work with vectors, matrices, and tensors

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- Computers are great with numbers (scalars)
- Domain experts work with vectors, matrices, and tensors
- Computers are not (yet?) great with those
- Lots of (very good) libraries for specific operations exist
- Is that enough? Sometimes

Libraries: back to the '70s!

- 1971: NAG Fortran Library – scientific computing
- 1972: EISPACK – eigenproblems
- 1973: BLAS 1 – basic vector ops
- 1975: LINPACK – linear systems
- ...
- ...

Approach

1. Identify a bottleneck
   e.g., linear system, eigenproblem, least-squares problem, SVD, ...

2. Encapsulate into a function
   e.g., `dgesv`, `dsyevd`, `dgelsx`, `dgesvd`, ...

3. Optimize, specialize

Basic linear algebra operations – 1973

"[..] a fairly small number of basic operations which are generally **responsible for a significant percentage** *of the total execution time"* – Hanson, Krogh, Lawson

- DOT: $\boldsymbol{w} := \boldsymbol{x}^T \boldsymbol{y}$ → DOT
- ELVOP: $\boldsymbol{y} := \alpha \boldsymbol{x} + \boldsymbol{y}$ → AXPY
- NRM: $\eta := (\boldsymbol{x}^T \boldsymbol{x})^{1/2}$ → NORM

1973 – 1979

- 1973: *"A proposal for standard linear algebra subprograms"* – Hanson, Krogh, Lawson
  Class I: DOT, ELVOP, G2, MG2 – Assembly
  Class II: NRM, XDOT, COPY, SWAP, SCALE, SUM, MAX – Fortran
- 1974: *"Standardization of FORTRAN callable subprograms for basic linear algebra"* – Lawson
- 1975–: LINPACK
- 1977: *"Basic Linear Algebra Subprograms for FORTRAN usage—an extended report"* – Hanson, Krogh, Kinkaid, Lawson
- 1977: *"Fortran BLAS timing"* – Dongarra
  Tests on 24 different computers

1979: BLAS 1

"Basic Linear Algebra Subprograms for FORTRAN usage"
— Hanson, Krogh, Kinkaid, Lawson (ACM TOMS)

"38 subprograms for basic operations of linear algebra"

- "aid in **design** and **coding** stages"
- "self-**documenting** quality of code"
- "a reduction of the execution time spent in these operations might be reflected in **cost savings** in the running of programs"
- "the programming of some of these low level operations involves **algorithmic and implementation subtleties** that are likely to be ignored"

Libraries

1970s

- Identification, analysis, optimization of **building blocks**

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  BUT
  Programs “easy” to optimize
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since 1980s

- Increasingly complex HW:
  E.g., vector processors, memory hierarchies, prefetching, ...

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  Programs difficult to optimize
- Cost($\mathcal{Alg}$) $\not\equiv$ #operations($\mathcal{Alg}$)
- **Libraries**: as before +
  necessity for performance

- 1988: BLAS 2 *"with some modern machine architectures, the use of the BLAS is not the best way to improve the efficiency of higher level codes. [..] the use of BLAS inhibits this optimization."*

  Matrix-vector operations **NOT** built on top of BLAS 1

- 1990: BLAS 3 *"Unfortunately, [BLAS 2] is often not well suited to computers with a hierarchy of memory"*

  Matrix-matrix operations **NOT** built on top of BLAS 1 & 2

- Immediate, widespread adoption: LAPACK, ScaLAPACK, PETSc, PLAPACK, ...

- Specialization, optimization, auto-tuning, high-level notation, automation, ...

Linear Algebra Libraries: 1970s

"Basic Linear Algebra Subprograms for FORTRAN usage", ACM TOMS, 1979

BLAS-1

Linear Algebra Libraries: 1980s

BLAS-2: Mat-vec ops, ACM TOMS 1988. BLAS-3: mat-mat ops, ACM TOMS 1990

BLAS-1, BLAS-2, BLAS-3

Linear Algebra Libraries: 1990s

Solvers & eigensolvers, 1992

LAPACK

BLAS-1, BLAS-2, BLAS-3

Linear Algebra Libraries: 1990s

Distributed Memory, 1995, 1997

ScaLAPACK, PLAPACK, ...

LAPACK

BLAS-1, BLAS-2, BLAS-3

Linear Algebra Libraries: 1990s

Dense & Sparse, 1997

PETSc, ...

ScaLAPACK, PLAPACK, ...

LAPACK

BLAS-1, BLAS-2, BLAS-3

Linear Algebra Libraries

and more!

PETSc, Trilinos, ...

ScaLAPACK, PLAPACK, Elemental, ...

LAPACK, Plasma, SuperMatrix, Magma, ...

BLAS-1, BLAS-2, BLAS-3, ATLAS, BTO-BLAS, BLIS, ...

Lin.alg. software landscape

Salient features

- Mature, expansive
- Community effort
- Standardized interface
- Careful organization: support routines, linear-systems, eigen-decompositions
- Clear layering: functionality, parallelism
- Well documented
- Performance-driven & HW-driven development

ACM Turing Award

ACM Turing Award

JACK DONGARRA

United States – 2021

CITATION

For his pioneering contributions to numerical algorithms and libraries that enabled high performance computational software to keep pace with exponential hardware improvements for over four decades

RESEARCH SUBJECTS

Approach - ?

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As opposed to what?

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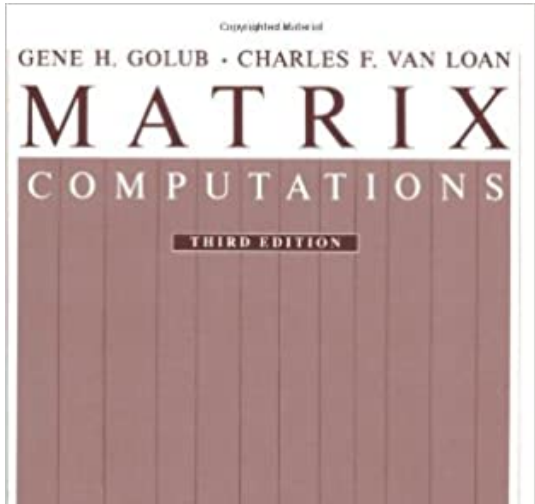
3. Optimize

As opposed to what? Workflow! Iteration vs. loop as a whole.

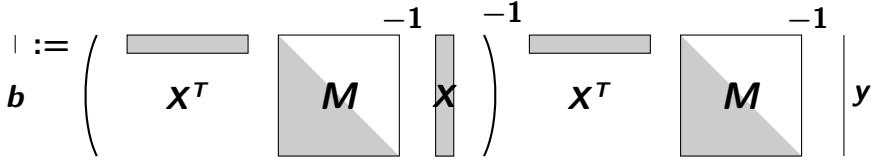
D. Fabregat, P. Bientinesi; ACM TOMS, 2014 [arXiv:1403.6426v1]
"Computing Petaflops over Terabytes of Data: The Case of Genome-Wide Association Studies"

C. Psarras, L. Karlsson, R. Bro, P. Bientinesi; ACM TOMS, 2022 [arXiv:2010.04678v2]
"Concurrent Alternating Least Squares for multiple simultaneous Canonical Polyadic Decompositions"

There is a matrix at your door



$$b := \left(X^T M^{-1} X\right)^{-1} X^T M^{-1} y$$



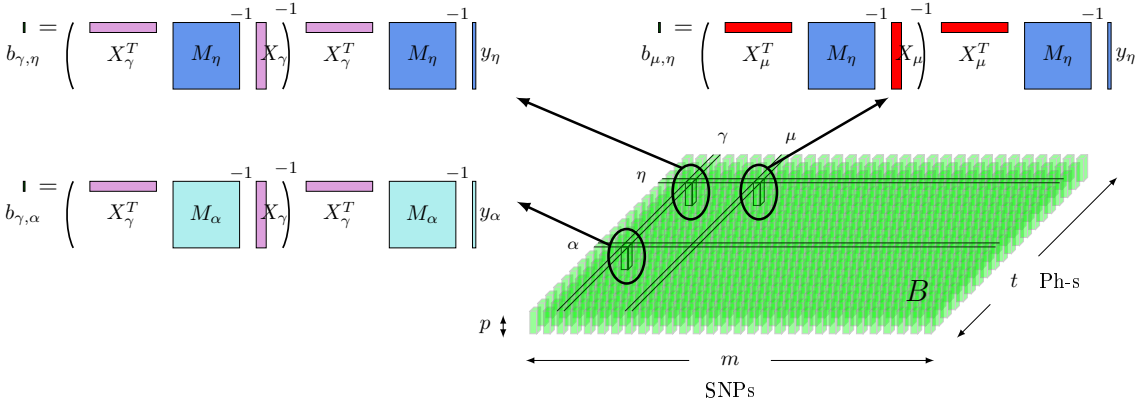
- $X \in \mathcal{R}^{n \times p}$ "SNP"
- $y \in \mathcal{R}^{n}$ "trait"
- $b \in \mathcal{R}^{p}$ "genetic effect"
- $M \in \mathcal{R}^{n \times n}$ "covariance matrix"

- $n \approx 1{,}000 - 50{,}000$
- $p \in [1, ..., 20]$
- M: SPD

"To be repeated millions of times"

Problem as a whole

$$\boldsymbol{b_{ij} := \left(X_i^T M_j^{-1} X_i\right)^{-1} X_i^T M_j^{-1} y_j}$$



Matrix computations

Signal Processing	$x := \left(A^{-T}B^TBA^{-1} + R^TLR\right)^{-1} A^{-T}B^TBA^{-1}y$	$R \in \mathbb{R}^{n-1\times n}$, UT; $L \in \mathbb{R}^{n-1\times n-1}$, DI
Kalman Filter	$K_k := P_k^bH^T(HP_k^bH^T + R)^{-1};\ x_k^a := x_k^b + K_k(z_k - Hx_k^b);\ P_k^a := (I - K_KH)\,P_k^b$	
Ensemble Kalman Filter	$X^a := X^b + \left(B^{-1} + H^TR^{-1}H\right)^{-1}\left(Y - HX^b\right)$	$B \in \mathbb{R}^{N\times N}$ SSPD; $R \in \mathbb{R}^{m\times m}$, SSPD
Ensemble Kalman Filter	$\delta X := \left(B^{-1} + H^TR^{-1}H\right)^{-1}H^TR^{-1}\left(Y - HX^b\right)$	
Ensemble Kalman Filter	$\delta X := XV^T\left(R + HX(HX)^T\right)^{-1}\left(Y - HX^b\right)$	
Image Restoration	$x_k := (H^TH + \lambda\sigma^2I_n)^{-1}(H^Ty + \lambda\sigma^2(v_{k-1} - u_{k-1}))$	
Image Restoration	$H^\dagger := H^T(HH^T)^{-1};\ y_k := H^\dagger y + (I_n - H^\dagger H)x_k$	
Rand. Matrix Inversion	$X_{k+1} := S(S^TAS)^{-1}S^T + (I_n - S(S^TAS)^{-1}S^TA)X_k(I_n - AS(S^TAS)^{-1}S^T)$	
Rand. Matrix Inversion	$X_{k+1} := X_k + WA^TS(S^TAWA^TS)^{-1}S^T(I_n - AX_k)$	$W \in \mathbb{R}^{n\times n}$, SPD
Rand. Matrix Inversion	$X_{k+1} := X_k + (I_n - X_kA^T)S(S^TA^TWAS)^{-1}S^TA^TW$	
Rand. Matrix Inversion	$\Lambda := S(S^TAWAS)^{-1}S^T;\ \Theta := \Lambda AW;\ M_k := X_kA - I$ $X_{k+1} := X_k - M_k\Theta - (M_k\Theta)^T + \Theta^T(AX_kA - A)\Theta$	

Matrix computations (2)

Generalized Least Squares	$b := (X^T M^{-1} X)^{-1} X^T M^{-1} y$	$n > m$; $M \in \mathbb{R}^{n \times n}$, SPD; $X \in \mathbb{R}^{n \times m}$; $y \in \mathbb{R}^{n \times 1}$
Stochastic Newton	$B_k := \frac{k}{k-1} B_{k-1}(I_n - A^T W_k((k-1)I_l + W_k^T A B_{k-1} A^T W_k)^{-1} W_k^T A B_{k-1})$	
Optimization	$x_f := WA^T(AWA^T)^{-1}(b - Ax)$; $x_o := W(A^T(AWA^T)^{-1}Ax - c)$	
Optimization	$x := W(A^T(AWA^T)^{-1}b - c)$	
Triangular Matrix Inv.	$X_{10} := L_{10}L_{00}^{-1}$; $X_{20} := L_{20} + L_{22}^{-1}L_{21}L_{11}^{-1}L_{10}$; $X_{11} := L_{11}^{-1}$; $X_{21} := -L_{22}^{-1}L_{21}$	
Tikhonov Regularization	$x := (A^T A + \Gamma^T \Gamma)^{-1} A^T b$	$A \in \mathbb{R}^{n \times m}$; $\Gamma \in \mathbb{R}^{m \times m}$; $b \in \mathbb{R}^{n \times 1}$
Tikhonov Regularization	$x := (A^T A + \alpha^2 I)^{-1} A^T b$	
Gen. Tikhonov Reg.	$x := (A^T PA + Q)^{-1}(A^T Pb + Qx_0)$	$P \in \mathbb{R}^{n \times n}$, SSPD; $Q \in \mathbb{R}^{m \times m}$, SSPD; $x_0 \in \mathbb{R}^{m \times 1}$
Gen. Tikhonov reg.	$x := x_0 + (A^T PA + Q)^{-1}(A^T P(b - Ax_0))$	
LMMSE estimator	$K_{t+1} := C_t A^T (AC_t A^T + C_z)^{-1}$; $x_{t+1} := x_t + K_{t+1}(y - Ax_t)$; $C_{t+1} := (I - K_{t+1}A)C_t$	
LMMSE estimator	$x_{\text{out}} = C_X A^T (AC_X A^T + C_Z)^{-1}(y - Ax) + x$	
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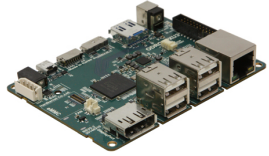
$$K_k := P_k^b H^T (H P_k^b H^T + R)^{-1}; \quad x_k^a := x_k^b + K_k(z_k - H x_k^b); \quad P_k^a := (I - K_K H)\, P_k^b$$

$$\begin{cases} C_\dagger := PCP^T + Q \\ K := C_\dagger H^T (H C_\dagger H^T)^{-1} \end{cases}$$

$$\Lambda := S(S^T AWAS)^{-1} S^T; \; \Theta := \Lambda AW; \; M_k := X_k A - I$$
$$X_{k+1} := X_k - M_k \Theta - (M_k \Theta)^T + \Theta^T (A X_k A - A)\Theta$$

$$x := A(B^T B + A^T R^T \Lambda R A)^{-1} B^T B A^{-1} y \quad \ldots \quad E := Q^{-1} U (I + U^T Q^{-1} U)^{-1} U^T$$



MUL | ADD | MOV

MOVAPD

VFMADDPD ...

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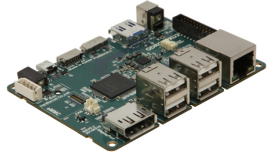

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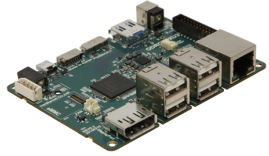
?

2-step solution



MUL | ADD | MOV

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Step 1: Libraries of building blocks

Support for all kinds of matrix types, parallelism, and platforms

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Support for all kinds of matrix types, parallelism, and platforms

PETSc, Trilinos, ...

ScaLAPACK, PLAPACK, Elemental, ...

LAPACK, Plasma, SuperMatrix, Magma, ...

BLAS-1, BLAS-2, BLAS-3, ATLAS, BTO-BLAS, BLIS, ...

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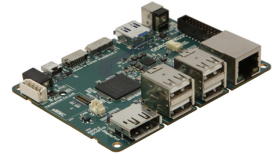
$$x := A(B^T B + A^T R^T \Lambda R A)^{-1} B^T B A^{-1} y \quad \ldots \quad E := Q^{-1}U(I + U^T Q^{-1} U)^{-1} U^T$$

$$y := \alpha x + y \qquad LU = A \qquad \cdots \qquad C := \alpha AB + \beta C$$

$$X := A^{-1}B \qquad C := AB^T + BA^T + C \qquad X := L^{-1}ML^{-T} \qquad QR = A$$

... **BLAS** **LAPACK** ...



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$$\Lambda := S(S^T AWAS)^{-1} S^T; \ \Theta := \Lambda AW; \ M_k := X_k A - I$$
$$X_{k+1} := X_k - M_k\Theta - (M_k\Theta)^T + \Theta^T(AX_kA - A)\Theta$$

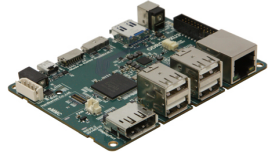
$$x := A(B^TB + A^TR^T\Lambda RA)^{-1}B^TBA^{-1}y \quad \ldots \quad E := Q^{-1}U(I + U^TQ^{-1}U)^{-1}U^T$$

?

$y := \alpha x + y$ | $LU = A$ | $\cdots$ | $C := \alpha AB + \beta C$

$X := A^{-1}B$ | $C := AB^T + BA^T + C$ | $X := L^{-1}ML^{-T}$ | $QR = A$

... BLAS LAPACK ...



MUL | ADD | MOV

MOVAPD

VFMADDPD ...

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$$x := A(B^T B + A^T R^T \Lambda R A \quad\quad -1 U (I + U^T Q^{-1} U)^{-1} U^T$$

Step 2:
LINEAR ALGEBRA MAPPING PROBLEM ("LAMP")

$$y := \alpha x + y \qquad LU = A \qquad \cdots \qquad C := \alpha AB + \beta C$$
$$X := A^{-1} B \qquad C := AB^T + BA^T + C \qquad X := L^{-1} M L^{-T} \qquad QR = A$$

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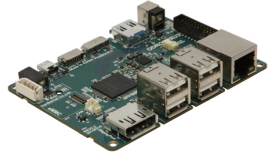

MUL ADD MOV
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... BLAS LAPACK ...

C. Psarras, H. Barthels, P. Bientinesi, [arXiv:1911.09421]
"The Linear Algebra Mapping Problem. Current state of linear algebra languages and libraries", ACM TOMS, 2022

A. Sankaran, N.A. Alashti, C. Psarras, P. Bientinesi, [arXiv:2202.09888]
"Benchmarking the Linear Algebra Awareness of TensorFlow and PyTorch", iWAPT-22

H. Barthels, C. Psarras, P. Bientinesi, [arXiv:1912.12924]
"Linnea: Automatic Generation of Efficient Linear Algebra Programs", ACM TOMS, 2021

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Find a sequence of calls to building blocks in $\mathcal{K}$, optimal according to $\mathcal{M}$, that computes all the assignments in $\mathcal{E}$.

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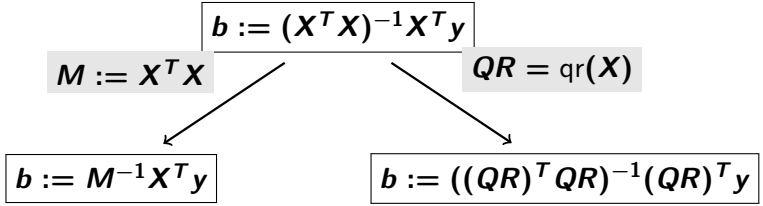
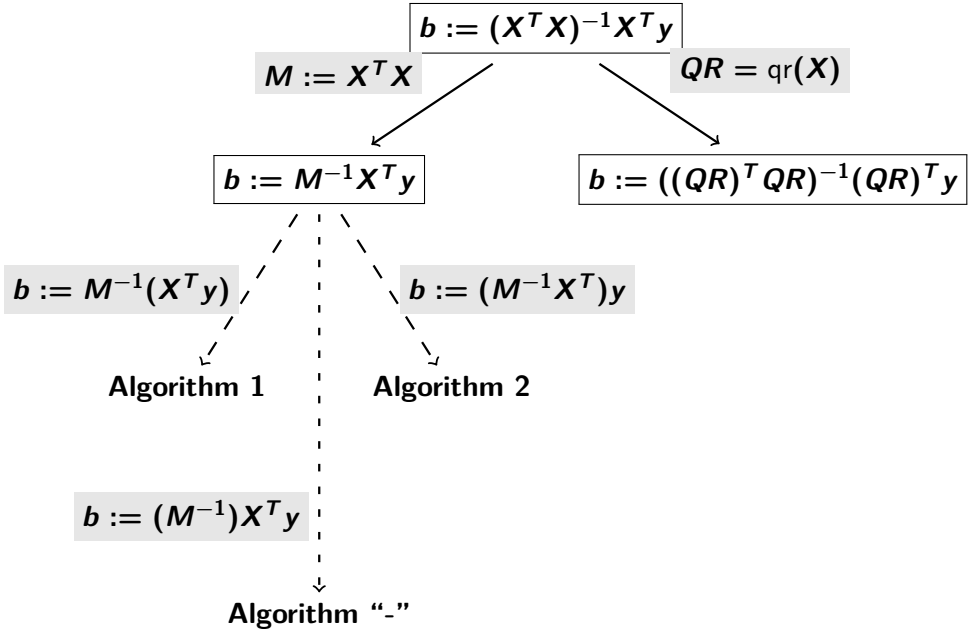
LAMP:
Find a sequence of calls to building blocks in $\mathcal{K}$, optimal according to $\mathcal{M}$, that computes all the assignments in $\mathcal{E}$.

- Suboptimal solution $\longrightarrow$ easy
- Optimality $\longrightarrow$ NP complete $\longleftarrow$ reduction from Ensemble Computation

$$\boxed{b := (X^T X)^{-1} X^T y}$$


$b := (X^T X)^{-1} X^T y$
$M := X^T X$
$QR = \text{qr}(X)$
$b := M^{-1} X^T y$
$b := ((QR)^T QR)^{-1} (QR)^T y$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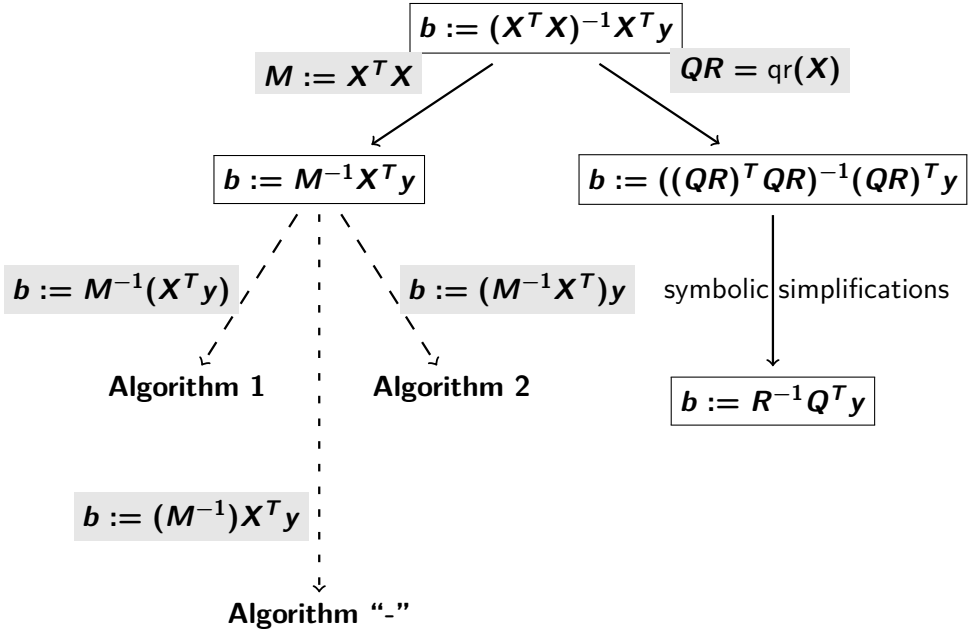
$b := M^{-1}(X^T y)$
$b := (M^{-1} X^T) y$
Algorithm 1
Algorithm 2
$b := (M^{-1}) X^T y$
Algorithm "-"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$b := (M^{-1} X^T) y$
symbolic simplifications
Algorithm 1
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$b := R^{-1} Q^T y$
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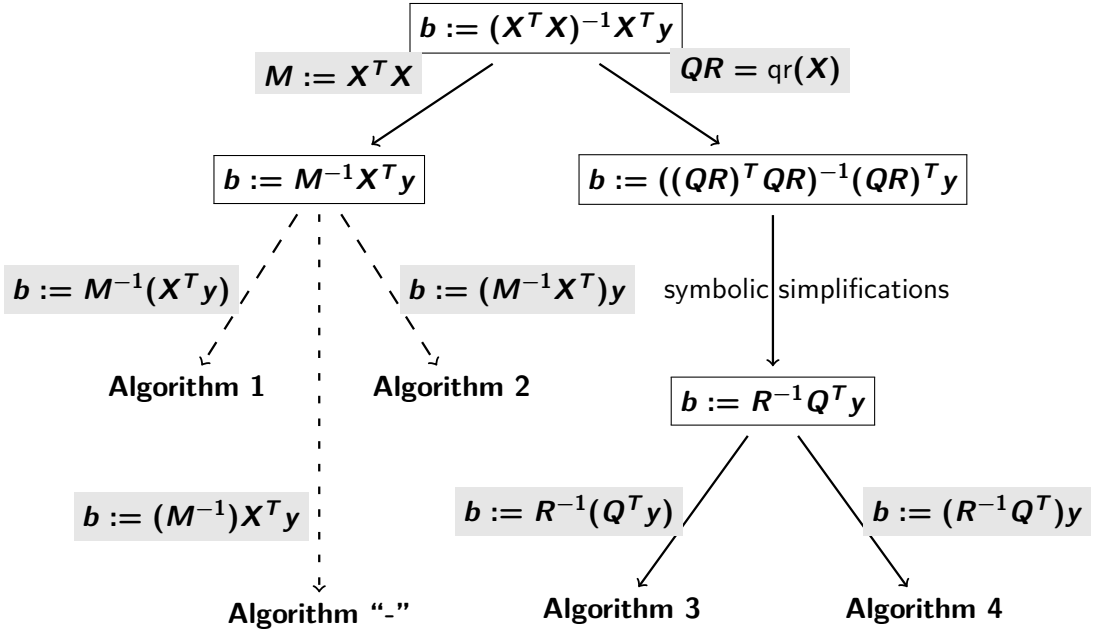
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$b := R^{-1} Q^T y$
$b := (M^{-1}) X^T y$
$b := R^{-1}(Q^T y)$
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Algorithm "-"
Algorithm 3
Algorithm 4

Problem acknowledged, yet overlooked

"How do users go about solving their matrix computations?"

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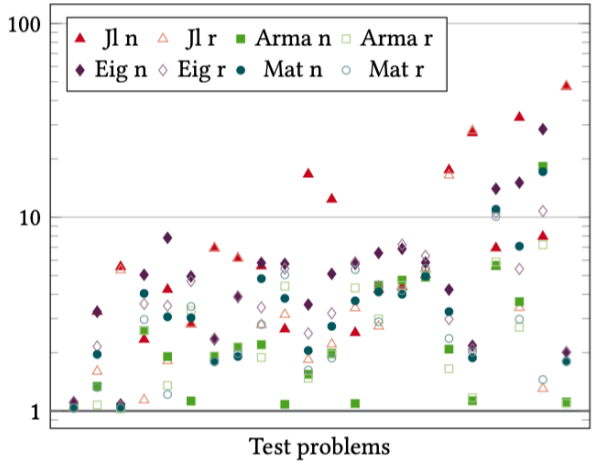
Computer efficiency?

Languages "slowdowns" wrt fast solutions – sequential execution



Jl: Julia, **Arma**: Armadillo, **Eig**: Eigen, **Mat**: Matlab. **n**/**r**: naive/recommended implementation

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Speedy development — slow solutions $\longrightarrow$ "2-language problem"

Investigation: How well do high-level languages solve LAMPs?

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Seven languages/libraries. Not an exhaustive survey.

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```
C = A * B'+ B * A' + C;                          // Matlab, Octave

C = A * transpose(B) + B * transpose(A) + C      // Julia

C = A * trans(B) + B * trans(A) + C;             // Armadillo

C = A * B.transpose() + B * A.transpose() + C;   // Eigen

ct = at @ bt.T + bt @ at.T + ct                  // NumPy

ct <- at %*% t(bt) + bt %*% t(at) + ct           // R
```

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C = A * trans(B) + B * trans(A) + C;             // Armadillo

C = A * B.transpose() + B * A.transpose() + C;   // Eigen

ct = at @ bt.T + bt @ at.T + ct                  // NumPy

ct <- at %*% t(bt) + bt %*% t(at) + ct           // R
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Investigation then adapted and extended to TensorFlow and PyTorch

Do they map? matrix products

	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
$C = AB$								

Do they map? matrix products

	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
$C = AB$	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27

Do they map? matrix products

	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
$C = AB$	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27
`GEMM`	✓	✓	✓	✓	✓	✓	✓	

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C = AB	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27
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C = C+AA'

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C = AB	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27
`GEMM`	✓	✓	✓	✓	✓	✓	✓	
C = C+AA'	0.18	0.17	0.21	0.32	0.29	0.17	0.18	0.14

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C = AB	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27
`GEMM`	✓	✓	✓	✓	✓	✓	✓	
C = C+AA'	0.18	0.17	0.21	0.32	0.29	0.17	0.18	0.14
`SYRK`	✓	✓	✓	×	×	✓	✓	

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C = AB	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27
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C = C+AA'	0.18	0.17	0.21	0.32	0.29	0.17	0.18	0.14
`SYRK`	✓	✓	✓	×	×	✓	✓	
C = C+AB'+BA'	0.57	0.59	0.69	0.59	0.58	0.57	0.58	0.28

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C = AB	0.29	0.28	0.30	0.31	0.29	0.29	0.29	0.27
`GEMM`	✓	✓	✓	✓	✓	✓	✓	
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`SYRK`	✓	✓	✓	×	×	✓	✓	
C = C+AB'+BA'	0.57	0.59	0.69	0.59	0.58	0.57	0.58	0.28
`SYR2K`	×	×	×	×	×	×	×	

Do they map? $\boldsymbol{Ax = b} \quad \equiv \quad \boldsymbol{x := A \backslash b} \quad \not\equiv \quad \text{inv}(\boldsymbol{A}) * \boldsymbol{b}$

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	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
$\boldsymbol{x := A \backslash b}$	0.71	0.72	0.63	0.68	0.64	0.63	0.72	0.61

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	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
$\boldsymbol{x := A \backslash b}$	0.71	0.72	0.63	0.68	0.64	0.63	0.72	0.61
$\text{inv}(\boldsymbol{A}) * \boldsymbol{b}$	1.76	1.82	1.69	2.20	2.21	**0.63**	2.49	1.71

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LinSolve	-	-	-	-	-	✓	-	-

but ...

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LinSolve	-	-	-	-	-	✓	-	-

but . . . should they map?

Remember

$\alpha, \beta, x \in \mathbf{R}, \quad A, B, C, X \in \mathbf{R^{m,n}}$

Commutativity($*$)

$$x := \alpha * \beta * \alpha^{-1} \quad \Rightarrow \quad x := \beta$$

$$X := A * B * A^{-1} \quad \not\Rightarrow \quad x := B$$

Remember

$\alpha, \beta, x \in \mathbf{R}, \quad \boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}, \boldsymbol{X} \in \mathbf{R}^{m,n}$

Commutativity($*$)

$$x := \alpha * \beta * \alpha^{-1} \quad \Rightarrow \quad x := \beta$$

$$\boldsymbol{X} := \boldsymbol{A} * \boldsymbol{B} * \boldsymbol{A}^{-1} \quad \not\Rightarrow \quad x := \boldsymbol{B}$$

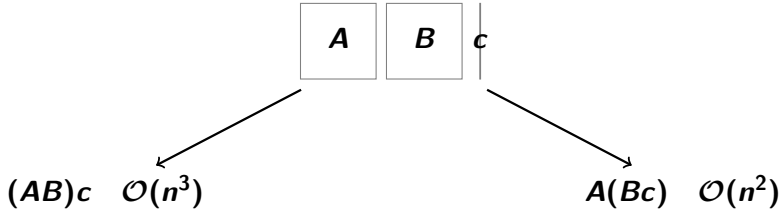
Associativity($*$)

$$\boldsymbol{X} := (\boldsymbol{A} * \boldsymbol{B}) * \boldsymbol{C} \quad \equiv \quad \boldsymbol{X} := \boldsymbol{A} * (\boldsymbol{B} * \boldsymbol{C})$$

But

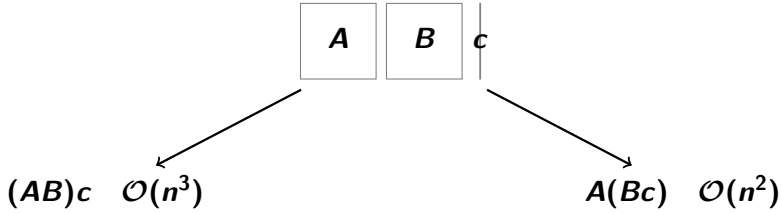
$$\text{Cost}\,((\boldsymbol{A} * \boldsymbol{B}) * \boldsymbol{C}) \quad \not\equiv \quad \text{Cost}\,(\boldsymbol{A} * (\boldsymbol{B} * \boldsymbol{C}))$$

Optimal parenthesisation



Matrix product is associative, but its cost is not

Optimal parenthesisation



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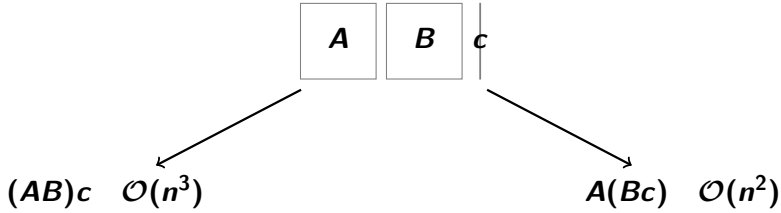
Matrix Chain(k)

Which is the best one?

Catalan$(k-1)$ parenthesiszations
if parallelism, then $k!$ parenthesiszations

Optimal parenthesisation



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Catalan$(k-1)$ parenthesiszations
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Which is the best one?

Matrix Chain Algorithm(k)

$O(k \log k)$ Hu & Shing 1982
$O(k^3)$ dynamic programming

Matrix Chain?

Chain	**Optimal Evaluation**
1) “left-to-right” (LtR)	((A B) C)
2) “right-to-left” (RtL)	(A (B C))
3) “mixed” (Mix)	((A B) (C D))

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3) "mixed" (Mix)	((A B) (C D))

		Matlab	Octave	Julia	R	Eigen	Armad.	NumPy
1)	LtR no par.	0.056	0.056	0.055	0.061	0.058	0.056	0.055
	LtR guided	0.056	0.056	0.055	0.061	0.058	0.056	0.055

Matrix Chain?

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1) "left-to-right" (LtR)	((A B) C)
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		Matlab	Octave	Julia	R	Eigen	Armad.	NumPy
1)	LtR no par.	0.056	0.056	0.055	0.061	0.058	0.056	0.055
	LtR guided	0.056	0.056	0.055	0.061	0.058	0.056	0.055
2)	RtL no par.	0.42	0.43	0.42	0.44	0.42	**0.055**	0.42
	RtL guided	0.055	0.056	0.054	0.059	0.056	0.055	0.056

Matrix Chain?

Chain	**Optimal Evaluation**
1) "left-to-right" (LtR)	((A B) C)
2) "right-to-left" (RtL)	(A (B C))
3) "mixed" (Mix)	((A B) (C D))

		Matlab	Octave	Julia	R	Eigen	Armad.	NumPy
1)	LtR no par.	0.056	0.056	0.055	0.061	0.058	0.056	0.055
	LtR guided	0.056	0.056	0.055	0.061	0.058	0.056	0.055
2)	RtL no par.	0.42	0.43	0.42	0.44	0.42	**0.055**	0.42
	RtL guided	0.055	0.056	0.054	0.059	0.056	0.055	0.056
3)	Mix no par.	0.32	0.33	0.33	0.33	0.35	0.31	0.33
	Mix guided	0.21	0.22	0.22	0.22	0.23	0.20	0.22

Matrix Chain?

Chain	Optimal Evaluation
1) "left-to-right" (LtR)	((A B) C)
2) "right-to-left" (RtL)	(A (B C))
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		Matlab	Octave	Julia	R	Eigen	Armad.	NumPy
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	LtR guided	0.056	0.056	0.055	0.061	0.058	0.056	0.055
2)	RtL no par.	0.42	0.43	0.42	0.44	0.42	**0.055**	0.42
	RtL guided	0.055	0.056	0.054	0.059	0.056	0.055	0.056
3)	Mix no par.	0.32	0.33	0.33	0.33	0.35	0.31	0.33
	Mix guided	0.21	0.22	0.22	0.22	0.23	0.20	0.22
	Matrix chains	×	×	×	×	×	≈	×

Challenge: Generalized Matrix Chain

[arXiv:1804.04021]

Matrix chains in practice

- Unary operators: transposition, inversion ($\boldsymbol{X} := \boldsymbol{A}\boldsymbol{B}^T\boldsymbol{C}^{-T}\boldsymbol{D} + \dots$)
- Overlapping kernels (e.g., $\boldsymbol{L} \leftarrow \boldsymbol{L}^{-1}$, $\boldsymbol{X} = \boldsymbol{A}^{-1}\boldsymbol{B}$)
- Decompositions (e.g., $\boldsymbol{A} \rightarrow \boldsymbol{Q}^T\boldsymbol{D}\boldsymbol{Q}$, $\boldsymbol{A} \rightarrow \boldsymbol{L}\boldsymbol{U}$)
- Properties & specialized kernels (`GEMM`, `TRMM`, `SYMM`, ...)

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$\Rightarrow$ **Generalized** Matrix Chain Algorithm

Challenge: Not all flops were created equal

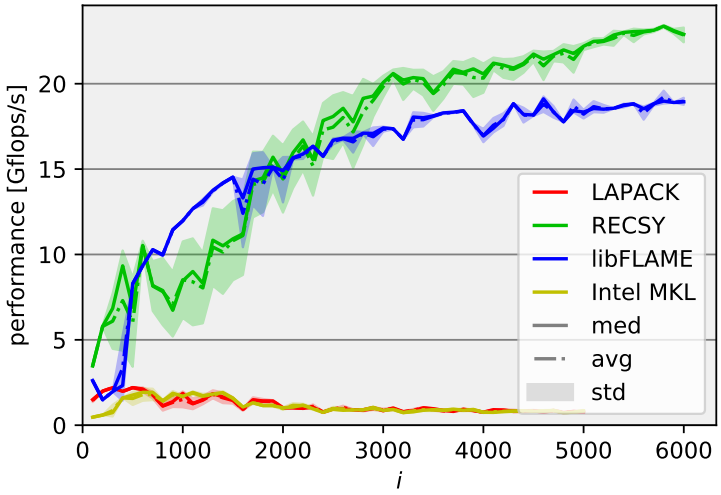
#FLOPs vs. execution time (vs. numerical stability)

$$\operatorname*{argmin}_{\mathcal{A}} \left(\text{FLOPs}(\mathcal{A}) \right) \neq \operatorname*{argmin}_{\mathcal{A}} \left(\text{time}(\mathcal{A}) \right)$$

Challenge: Not all flops were created equal

[arXiv:1504.08035]

Triangular Sylvester equation – all libraries perform the same # of flops



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[arXiv:1706.01341]

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Big Challenge: **Parallelism**

$$\boldsymbol{X} := \boldsymbol{A}((\boldsymbol{B}^T\boldsymbol{C}^{-T})\boldsymbol{D}) \quad \text{vs.} \quad \boldsymbol{X} := (\boldsymbol{A}\boldsymbol{B}^T)(\boldsymbol{C}^{-T}\boldsymbol{D}) \quad \text{vs.} \quad \ldots$$

Properties?

Operation	Property	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
Linear System	-	0.71	0.74	0.62	0.67	0.63	0.62	0.65	0.61

Properties?

Operation	Property	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
Linear System	-	0.71	0.74	0.62	0.67	0.63	0.62	0.65	0.61
	Symmetric	0.71	0.73	0.62	0.69	N/A	0.62	0.65	0.46

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Operation	Property	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
Linear System	-	0.71	0.74	0.62	0.67	0.63	0.62	0.65	0.61
	Symmetric	0.71	0.73	0.62	0.69	N/A	0.62	0.65	0.46
	SPD	**0.41**	**0.40**	0.60	0.63	N/A	**0.34**	0.62	0.31

Properties?

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Linear System	-	0.71	0.74	0.62	0.67	0.63	0.62	0.65	0.61
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	SPD	**0.41**	**0.40**	0.60	0.63	N/A	**0.34**	0.62	0.31
	Triangular	**0.03**	**0.04**	**0.03**	0.63	N/A	0.62	0.65	0.03

Properties?

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Linear System	-	0.71	0.74	0.62	0.67	0.63	0.62	0.65	0.61
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	Triangular	**0.03**	**0.04**	**0.03**	0.63	N/A	0.62	0.65	0.03
	Diagonal	0.03	0.05	**0.01**	0.63	N/A	**0.03**	0.62	0.001
		$\approx$	$\approx$	$\approx$	$\times$	$\times$	$\approx$	$\times$	

Properties?

Operation	Property	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy	C
Linear System	-	0.71	0.74	0.62	0.67	0.63	0.62	0.65	0.61
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	SPD	**0.41**	**0.40**	0.60	0.63	N/A	**0.34**	0.62	0.31
	Triangular	**0.03**	**0.04**	**0.03**	0.63	N/A	0.62	0.65	0.03
	Diagonal	0.03	0.05	**0.01**	0.63	N/A	**0.03**	0.62	0.001
		$\approx$	$\approx$	$\approx$	$\times$	$\times$	$\approx$	$\times$	
Multiplication	-	1.44	1.48	1.47	1.47	1.45	1.44	1.44	1.46
	Triangular	1.44	1.48	**0.75**	1.47	1.45	1.44	1.44	0.74
	Diagonal	1.44	1.48	**0.03**	1.47	1.45	1.42	1.44	0.06
		$\times$	$\times$	✓	$\times$	$\times$	$\times$	$\times$	

Challenge: Inference of properties

- **easy** $\quad E := L_1 * U^T * L_2 \quad$ triangular(E) ?

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$\Rightarrow$ **Symbolic analysis**: pattern matching

Challenge: Common Subexpressions

[arXiv:1710.06915]

$$\begin{cases} X := AB^{-T}C \\ Y := B^{-1}A^{T}D \end{cases} \quad \rightarrow \quad \begin{cases} Z := AB^{-T} \\ X := ZC \\ Y := Z^{T}D \end{cases}$$

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BUT

$$X := ABABv \quad \not\rightarrow \quad \begin{cases} Z := AB \\ X := ZZv \end{cases}$$

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	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy
copy	0.27	0.31	0.36	0.30	0.30	0.26	0.30

Common Subexpressions?

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	Matlab	Octave	Julia	R	Eigen	Armad.	NumPy
copy	0.27	0.31	0.36	0.30	0.30	0.26	0.30
direct	0.54	0.6	0.61	0.56	0.58	0.52	0.55
	×	×	×	×	×	×	×

Other features (challenges)

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$$M = \begin{bmatrix} M_1 & 0 \\ 0 & M_2 \end{bmatrix}$$

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- $\mathrm{diag}(\boldsymbol{A} + \boldsymbol{B})$ vs. $\mathrm{diag}(\boldsymbol{A}) + \mathrm{diag}(\boldsymbol{B})$

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  $\mathrm{diag}(\boldsymbol{AB})$ vs. ...

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- Next: "**Linnea**: A linear algebra compiler" [arXiv:1912.12924]

Linnea

`https://linnea.cs.umu.se/`

Linnea

Linear algebra knowledge: operators, identities, properties, theorems

- Distributivity, commutativity, partitionings, ...
- Matrix chains, generalize matrix chains
- $((QR)^T QR)^{-1}(QR)^T y \;\rightarrow\; (R^T Q^T QR)^{-1} R^T Q^T y \;\rightarrow\; R^{-1} R^{-T} R^T Q^T y \;\rightarrow\; R^{-1} Q^T y$
- $\mathrm{SPD}(A) \rightarrow \mathrm{SPD}(A_{BR} - A_{BL} A_{TL}^{-1} A_{BL}^T)$ Schur complement
- ...

Linnea: Example

$$\boldsymbol{w} := \boldsymbol{A}\boldsymbol{B}^{-1}\boldsymbol{c}, \quad \text{SPD}(\boldsymbol{B})$$

Naive

```
w = A*inv(B)*c
```

Recommended

```
w = A*(B\c)
```

Expert

```
L = Chol(B)
w = A*(L'\(L\c))
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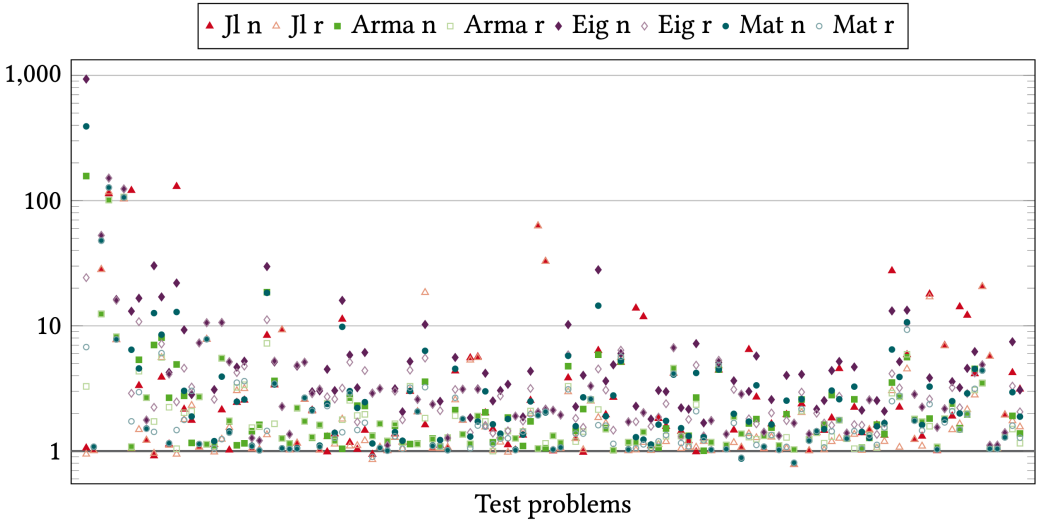
Generated

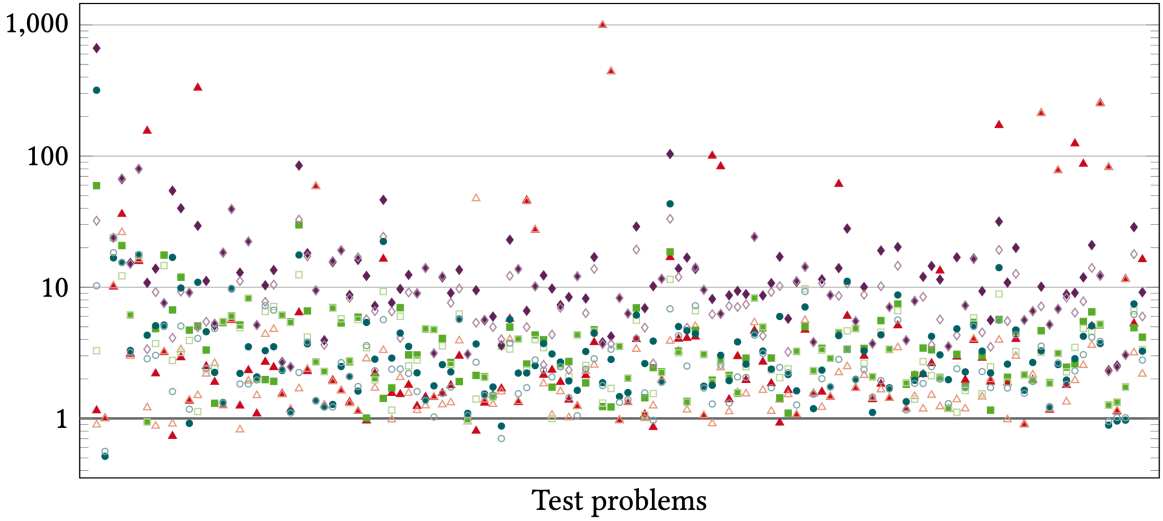
```
ml0 = A; ml1 = B; ml2 = c;
potrf!('L', ml1)
trsv!('L', 'N', 'N', ml1, ml2)
trsv!('L', 'T', 'N', ml1, ml2)
ml3 = Array{Float64}(10)
gemv!('N', 1.0, ml0, ml2, 0.0, ml3)
w = ml3
```

Linnea speedup: 1 thread



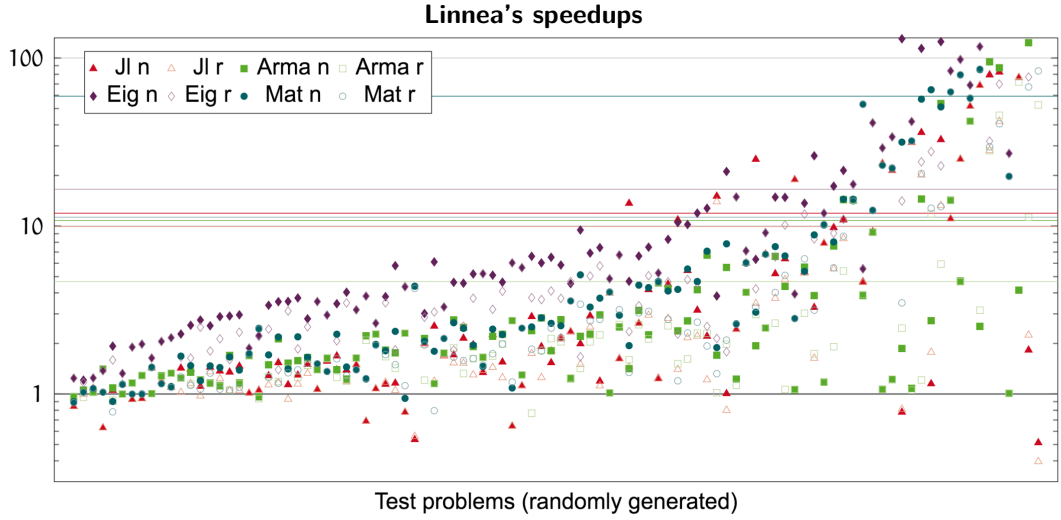
Jl: Julia, **Arma**: Armadillo, **Eig**: Eigen, **Mat**: Matlab. **n**/**r**: naive/recommended implementation

Linnea speedup: 24 threads



Jl: Julia, **Arma**: Armadillo, **Eig**: Eigen, **Mat**: Matlab. **n**/**r**: naive/recommended implementation

Linnea: Results for random expressions



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What's next?

-
-
-

What's next?

-
-
-

THANK YOU!!

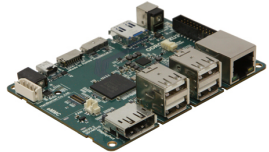
Tensor-land

Quantum Chemistry | High-order FEM | DG | ... | Tensor App #N

Transposition | Contraction | ... | Alternating LS

Khatri-Rao | SpMTTKRP | ... | TTV, TTM

HPTT **TCL** **...** **BLAS**



MUL | ADD | MOV

MOVAPD

VFMADDPD | ...