

Strassen-like algorithms for symmetric tensor contractions

Edgar Solomonik

University of Illinois at Urbana-Champaign

Scientific and Statistical Computing Seminar
University of Chicago

April 13, 2017

- 1 Introduction
- 2 Applications of tensor symmetry
- 3 Exploiting symmetry in matrix products
- 4 Exploiting symmetry in tensor contractions
- 5 Numerical error analysis
- 6 Exploiting partial-symmetry in tensor contractions
- 7 Communication cost analysis
- 8 Summary and conclusion

Terminology

A tensor $\mathbf{T} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ has

- order d (i.e. d modes / indices)
- dimensions n_1 -by- \dots -by- n_d (in this talk, usually each $n_i = n$)
- elements $\mathbf{T}_{i_1 \dots i_d} = T_{\mathbf{i}}$ where $\mathbf{i} \in \{1, \dots, n\}^d$

We say a tensor is **symmetric** if for any $j, k \in \{1, \dots, n\}$

$$\mathbf{T}_{i_1 \dots i_j \dots i_k \dots i_d} = \mathbf{T}_{i_1 \dots i_k \dots i_j \dots i_d}$$

A tensor is **antisymmetric** (skew-symmetric) if for any $j, k \in \{1, \dots, n\}$

$$\mathbf{T}_{i_1 \dots i_j \dots i_k \dots i_d} = (-1) \mathbf{T}_{i_1 \dots i_k \dots i_j \dots i_d}$$

A tensor is **partially-symmetric** if such index interchanges are restricted to be within subsets of $\{1, \dots, n\}$, e.g.

$$\mathbf{T}_{kl}^{ij} = \mathbf{T}_{kl}^{ji} = \mathbf{T}_{lk}^{ji} = \mathbf{T}_{lk}^{ij}$$

Tensor contractions

We work with contractions of tensors

- \mathbf{A} of order $s + v$, and
- \mathbf{B} of order $v + t$ into
- \mathbf{C} of order $s + t$, defined as

$$C_{ij} = \sum_{k \in \{1, \dots, n\}^v} A_{ik} B_{kj}$$

- requires $O(\underbrace{s + t + v}_{\omega})$ multiplications and additions
- assumes an index ordering, but does not lose generality
- works with any symmetries of \mathbf{A} and \mathbf{B}
- is extensible to symmetries of \mathbf{C} via [symmetrization](#) (sum all permutations of modes in \mathbf{C} , denoted $[\mathbf{C}]_{ij}$)
- generalizes simple matrix operations, e.g.

$$\underbrace{(s, t, v) = (1, 0, 1)}_{\text{matrix-vector product}}$$

$$\underbrace{(s, t, v) = (1, 1, 0)}_{\text{vector outer product}}$$

$$\underbrace{(s, t, v) = (1, 1, 1)}_{\text{matrix-matrix product}}$$

Applications of symmetric tensor contractions

Symmetric and Hermitian matrix operations are part of the BLAS

- matrix-vector products: `symv` (`symm`), `hemv`, (`hemm`)
- symmetrized outer product: `syr2` (`syr2k`), `her2`, (`her2k`)
- these operations dominate symmetric/Hermitian diagonalization

Hankel matrices are order $2 \log_2(n)$ partially-symmetric tensors

$$\mathbf{H} = \begin{bmatrix} \mathbf{H}_{11} & \mathbf{H}_{21}^T \\ \mathbf{H}_{21} & \mathbf{H}_{22} \end{bmatrix}$$

where \mathbf{H}_{11} , \mathbf{H}_{21} , \mathbf{H}_{22} are also Hankel.

In general, **partially-symmetric** tensors are **nested symmetric** tensors

- a nonsymmetric matrix is a vector of vectors
- $\mathbf{T}_{kl}^{ij} = \mathbf{T}_{kl}^{ji} = \mathbf{T}_{lk}^{ji} = \mathbf{T}_{lk}^{ij}$ is a symmetric matrix of symmetric matrices

Applications of partially-symmetric tensor contractions

High-accuracy methods in computational quantum chemistry

- solve the multi-electron Schrödinger equation $\mathbf{H}|\Psi\rangle = E|\Psi\rangle$, where \mathbf{H} is a linear operator, but Ψ is a function of *all* electrons
- use wavefunction ansatz like $\Psi \approx \Psi^{(k)} = e^{\mathbf{T}^{(k)}}|\Psi^{(k-1)}\rangle$ where $\Psi^{(0)}$ is a determinant function and $\mathbf{T}^{(k)}$ is an order $2k$ tensor, acting as a multilinear excitation operator on the electrons
- are most commonly versions of **coupled-cluster** methods which use the above ansatz for $k \in \{2, 3, 4\}$ (CCSD, CCSDT, CCSDTQ)
- solve iteratively for $\mathbf{T}^{(k)}$, where each iteration has cost $O(n^{2k+2})$, dominated by contractions of partially antisymmetric tensors
- for example, a dominant contraction in CCSD ($k = 2$) is

$$\mathbf{z}_{i\bar{c}}^{a\bar{k}} = \sum_{b=1}^n \sum_{j=1}^n \mathbf{T}_{ij}^{ab} \cdot \mathbf{v}_{b\bar{c}}^{j\bar{k}}$$

where $\mathbf{T}_{ij}^{ab} = -\mathbf{T}_{ij}^{ba} = \mathbf{T}_{ji}^{ba} = -\mathbf{T}_{ji}^{ab}$. We'll show an algorithm that requires n^6 rather than $2n^6$ operations.

Symmetric matrix times vector

- Let \mathbf{b} be a vector of length n with elements in ϱ
- Let \mathbf{A} be an n -by- n symmetric matrix with elements in ϱ

$$\mathbf{A}_{ij} = \mathbf{A}_{ji}$$

- We multiply matrix \mathbf{A} by \mathbf{b} ,

$$\mathbf{c} = \mathbf{A} \cdot \mathbf{b}$$

$$c_i = \sum_{j=1}^n \underbrace{\mathbf{A}_{ij} \cdot \mathbf{b}_j}_{\text{nonsymmetric}}$$

- This usual form has cost (ignoring low-order terms here and later)

$$T_{\text{symv}}(\varrho, n) = \mu_{\varrho} \cdot n^2 + \nu_{\varrho} \cdot n^2$$

where μ_{ϱ} is the cost of multiplication and ν_{ϱ} of addition

Fast symmetric matrix times vector

We can perform `symv` using fewer element-wise multiplications,

$$c_i = \sum_{j=1}^n \underbrace{\mathbf{A}_{ij} \cdot (\mathbf{b}_i + \mathbf{b}_j)}_{\text{symmetric}} - \underbrace{\left(\sum_{j=1}^n \mathbf{A}_{ij} \right) \cdot \mathbf{b}_i}_{\text{requires only } n \text{ mults.}}$$

- $\mathbf{A}_{ij} \cdot (\mathbf{b}_i + \mathbf{b}_j)$ is symmetric, requires $\binom{n+1}{2}$ multiplications
- $\left(\sum_{j=1}^n \mathbf{A}_{ij} \right) \cdot \mathbf{b}_i$ may be computed with n multiplications
- The total cost of the new form is

$$T'_{\text{symv}}(\rho, n) = \mu_\rho \cdot \frac{1}{2}n^2 + \nu_\rho \cdot \frac{5}{2}n^2$$

- This formulation is cheaper when $\mu_\rho > 3\nu_\rho$
- Form `symm` the formulation is cheaper when $\mu_\rho > \nu_\rho$

Symmetric rank-2 update

Consider a rank-2 outer product of vectors \mathbf{a} and \mathbf{b} of length n into symmetric matrix \mathbf{C}

$$\mathbf{C} = \mathbf{a} \cdot \mathbf{b}^\top + \mathbf{b} \cdot \mathbf{a}^\top$$
$$\mathbf{C}_{ij} = \left[\mathbf{a} \cdot \mathbf{b}^\top \right]_{ij} \equiv \underbrace{\mathbf{a}_i \cdot \mathbf{b}_j}_{\text{nonsymmetric}} + \underbrace{\mathbf{a}_j \cdot \mathbf{b}_i}_{\text{permutation}}$$

Usually computed via the n^2 multiplications $\mathbf{a}_i \cdot \mathbf{b}_j$ with the cost

$$T_{\text{symr2}}(\varrho, n) = \mu_\varrho \cdot n^2 + \nu_\varrho \cdot n^2.$$

Fast symmetric rank-2 update

We may compute the rank-2 update via a symmetric intermediate quantity

$$\mathbf{C}_{ij} = \underbrace{(\mathbf{a}_i + \mathbf{a}_j) \cdot (\mathbf{b}_i + \mathbf{b}_j)}_{\text{symmetric}} - \underbrace{\mathbf{a}_i \cdot \mathbf{b}_i - \mathbf{a}_j \cdot \mathbf{b}_j}_{\text{requires only } n \text{ mults in total}}$$

- We can compute all $(\mathbf{a}_i + \mathbf{a}_j) \cdot (\mathbf{b}_i + \mathbf{b}_j)$ in $\binom{n+1}{2}$ multiplications
- The total cost is then given to leading order by

$$T'_{\text{syr2}}(\varrho, n) = \mu_{\varrho} \cdot \frac{1}{2}n^2 + \nu_{\varrho} \cdot \frac{5}{2}n^2.$$

- $T'_{\text{syr2}}(\varrho, n) < T_{\text{syr2}}(\varrho, n)$ when $\mu_{\varrho} > 3\nu_{\varrho}$
- $T'_{\text{syr2K}}(\varrho, n, K) < T_{\text{syr2K}}(\varrho, n, K)$ when $\mu_{\varrho} > \nu_{\varrho}$

Symmetrized product of symmetric matrices

Given symmetric matrices \mathbf{A} , \mathbf{B} of dimension n on non-associative commutative ring ϱ , we seek to compute the **anticommutator** of \mathbf{A} and \mathbf{B}

$$\mathbf{C} = \mathbf{A} \cdot \mathbf{B} + \mathbf{B} \cdot \mathbf{A}$$
$$C_{ij} = [\mathbf{A} \cdot \mathbf{B}]_{ij} \equiv \sum_{k=1}^n \underbrace{\mathbf{A}_{ik} \cdot \mathbf{B}_{jk}}_{\text{nonsymmetric}} + \sum_{k=1}^n \underbrace{\mathbf{A}_{jk} \cdot \mathbf{B}_{ik}}_{\text{permutation}}$$

The above equations require n^3 multiplications and n^3 adds for a total cost of

$$T_{\text{symmm}}(\varrho, n) = \mu_{\varrho} \cdot n^3 + \nu_{\varrho} \cdot n^3.$$

Note that the symmetrized product defines a non-associative commutative ring (the Jordan ring) over the set of symmetric matrices.

Fast symmetrized product of symmetric matrices

We can combine the ideas from the fast routines for `symv` and `syrrk`

$$\begin{aligned} \mathbf{C}_{ij} &= \sum_k \underbrace{(\mathbf{A}_{ij} + \mathbf{A}_{ik} + \mathbf{A}_{jk}) \cdot (\mathbf{B}_{ij} + \mathbf{B}_{ik} + \mathbf{B}_{jk})}_{\text{symmetric, requires } \binom{n+2}{3} \text{ mults}} \\ &\quad - \underbrace{\mathbf{A}_{ij} \cdot \left(\sum_k \mathbf{B}_{ij} + \mathbf{B}_{ik} + \mathbf{B}_{jk} \right)}_{\text{requires } \binom{n+1}{2} \text{ mults}} - \underbrace{\mathbf{B}_{ij} \cdot \left(\sum_k \mathbf{A}_{ij} + \mathbf{A}_{ik} + \mathbf{A}_{jk} \right)}_{\text{requires } \binom{n+1}{2} \text{ mults}} \\ &\quad - \underbrace{\sum_k \mathbf{A}_{ik} \cdot \mathbf{B}_{ik} - \sum_k \mathbf{A}_{jk} \cdot \mathbf{B}_{jk}}_{\text{requires } \binom{n+1}{2} \text{ mults}} \end{aligned}$$

The reformulation requires $\binom{n}{3}$ multiplications to leading order,

$$T'_{\text{symmm}}(\varrho, n) = \mu_\varrho \cdot \frac{1}{6}n^3 + \nu_\varrho \cdot \frac{5}{3}n^3,$$

which is faster than T_{symmm} when $\mu_\varrho > (4/5)\nu_\varrho$.

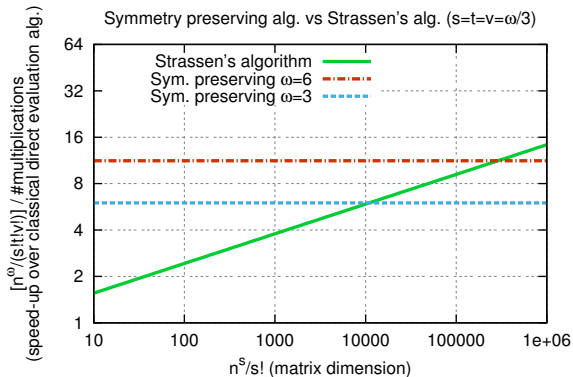
Fast symmetrized product of symmetric matrices

We can rewrite that algorithm in terms using symmetrization notation:

$$\begin{aligned} C_{ij} &= [\mathbf{AB}]_{ij} = \underbrace{\sum_k (\mathbf{A}_{ij} + \mathbf{A}_{ik} + \mathbf{A}_{jk}) \cdot (\mathbf{B}_{ij} + \mathbf{B}_{ik} + \mathbf{B}_{jk})}_{\sum_k [\mathbf{A}]_{ijk} \cdot [\mathbf{B}]_{ijk}} \\ &\quad - \underbrace{\mathbf{A}_{ij} \cdot \left(\sum_k \mathbf{B}_{ij} + \mathbf{B}_{ik} + \mathbf{B}_{jk} \right)}_{\mathbf{A}_{ij} \cdot \sum_k [\mathbf{B}]_{ijk}} - \underbrace{\mathbf{B}_{ij} \cdot \left(\sum_k \mathbf{A}_{ij} + \mathbf{A}_{ik} + \mathbf{A}_{jk} \right)}_{\mathbf{B}_{ij} \cdot \sum_k [\mathbf{A}]_{ijk}} \\ &\quad - \underbrace{\sum_k \mathbf{A}_{ik} \cdot \mathbf{B}_{ik} - \sum_k \mathbf{A}_{jk} \cdot \mathbf{B}_{jk}}_{[\mathbf{A}_{ik \circ 1} \mathbf{B}]_{ij}} \\ &= \sum_k [\mathbf{A}]_{ijk} \cdot [\mathbf{B}]_{ijk} - \mathbf{A}_{ij} \sum_k [\mathbf{B}]_{ijk} - \mathbf{B}_{ij} \sum_k [\mathbf{A}]_{ijk} - [\mathbf{A}_{\circ 1} \mathbf{B}]_{ij} \end{aligned}$$

where $\mathbf{A}_{\circ 1} \mathbf{B} = \sum_k \mathbf{A}_{ik} \cdot \mathbf{B}_{jk}$

Comparison to Strassen's algorithm



Fully symmetric tensor contractions

We can now state the general symmetric tensor contraction algorithms, given

- \mathbf{A} of order $s + v$, and
- \mathbf{B} of order $v + t$ into
- \mathbf{C} of order $s + t$, defined as

we define the (nonsymmetrized) contraction as $\mathbf{C} = \mathbf{A} \odot_v \mathbf{B}$ where

$$C_{ij} = \sum_{k \in \{1, \dots, n\}^v} A_{ik} B_{kj}$$

We can then define the symmetrized tensor contraction as

$$C_i = [\mathbf{A} \odot_v \mathbf{B}]_i$$

The usual method first computes $\mathbf{A} \odot_v \mathbf{B}$ with cost

$$T'_{\text{syctr}}(\varrho, n, s, t, v) = \mu_\varrho \cdot \binom{n}{s} \binom{n}{t} \binom{n}{v} + \nu_\varrho \cdot \binom{n}{s} \binom{n}{t} \binom{n}{v}.$$

Fast fully-symmetric contraction algorithm

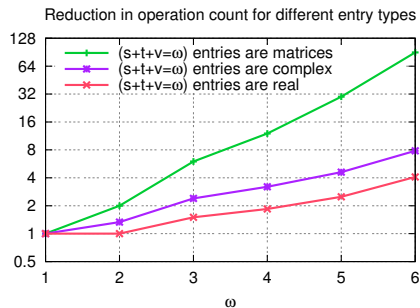
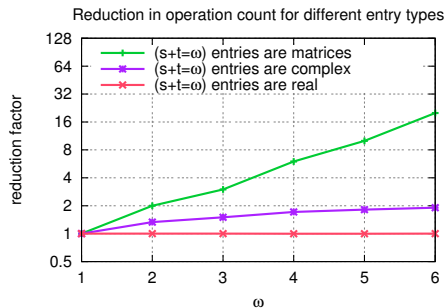
The fast algorithm is defined as follows (using $\omega = s + t + v$)

$$\begin{aligned} \mathbf{C}_i = & \underbrace{\sum_{\mathbf{k} \in \{1, \dots, n\}^v} [\mathbf{A}]_{ik} \cdot [\mathbf{B}]_{ik}}_{\text{symmetric, requires } \binom{n+\omega-1}{\omega} \text{ multiplications}} \\ & - \underbrace{\sum_{p+q=1}^v \sum_{\mathbf{k} \in \{1, \dots, n\}^{v-p-q}} \left(\sum_{\mathbf{p} \in \{1, \dots, n\}^p} [\mathbf{A}]_{ikp} \right) \cdot \left(\sum_{\mathbf{q} \in \{1, \dots, n\}^q} [\mathbf{B}]_{ikq} \right)}_{\text{requires } O(n^{\omega-1}) \text{ multiplications}} \\ & - \underbrace{\sum_{r=1}^{\min(s,t)} [\mathbf{A} \odot_{v+r} \mathbf{B}]_i}_{\text{requires } O(n^{\omega-1}) \text{ multiplications}} \end{aligned}$$

The leading order cost is

$$T'_{\text{syctr}}(\varrho, n, s, t, v) = \mu_{\varrho} \cdot \binom{n}{\omega} + \nu_{\varrho} \cdot \binom{n}{\omega} \cdot \left[\binom{\omega}{t} + \binom{\omega}{s} + \binom{\omega}{v} \right].$$

Reduction in operation count of fast algorithm with respect to standard



(s, t, v) values for left and right graph tabulated below

| ω | 1 | 2 | 3 | 4 | 4 | 6 |
|-------------|-----------|-----------|-----------|-----------|-----------|-----------|
| Left graph | (1, 0, 0) | (1, 1, 0) | (2, 1, 0) | (2, 2, 0) | (3, 2, 0) | (3, 3, 0) |
| Right graph | (1, 0, 0) | (1, 1, 0) | (1, 1, 1) | (2, 1, 1) | (2, 2, 1) | (2, 2, 2) |

Theoretical error bounds

We express error bounds in terms of $\gamma_n = \frac{n\epsilon}{1-n\epsilon}$, where ϵ is the machine precision.

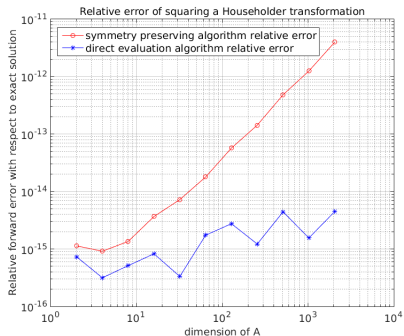
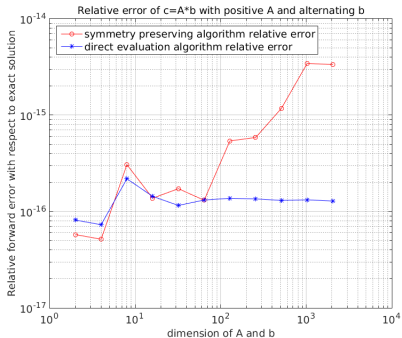
Let Ψ be the standard algorithm and Φ be the fast algorithm. The error bound for the standard algorithm arises from matrix multiplication

$$\|fl(\Psi(\mathbf{A}, \mathbf{B})) - \mathbf{C}\|_\infty \leq \gamma_m \cdot \|\mathbf{A}\|_\infty \cdot \|\mathbf{B}\|_\infty \quad \text{where } m = \binom{n}{v} \binom{\omega}{v}.$$

The following error bound holds for the fast algorithm

$$\|fl(\Phi(\mathbf{A}, \mathbf{B})) - \mathbf{C}\|_\infty \leq \gamma_m \cdot \|\mathbf{A}\|_\infty \cdot \|\mathbf{B}\|_\infty \quad \text{where } m = 3 \binom{n}{v} \binom{\omega}{t} \binom{\omega}{s}.$$

Stability of symmetry preserving algorithms



Nesting the fast algorithm

For partially-(anti)symmetric contractions we can

- nest the new algorithm over each group of symmetric modes
- reduction in mults can translate to reduction in the number of operations
- for Hankel matrices, yields sub $O(n^2)$ algorithm, but not $O(n)$ or $O(n \log(n))$ as reduction in mults is a factor of two only in leading order
- but for coupled-cluster contractions, significant reductions in cost can be achieved
 - CCSD 1.3X on a typical system
 - CCSDT 2.1X on a typical system
 - CCSDTQ 5.7X on a typical system

Communication cost of the standard algorithm

We consider communication bandwidth cost on a sequential machine with cache size M .

The intermediate formed by the standard algorithm may be computed via matrix multiplication with communication cost,

$$W(n, s, t, v, M) = \Theta \left(\frac{\binom{n}{s} \binom{n}{t} \binom{n}{v}}{\sqrt{M}} + \binom{n}{s+v} + \binom{n}{t+v} + \binom{n}{s+t} \right).$$

The cost of symmetrizing the resulting intermediate is low-order or the same.

Communication cost of the fast algorithm

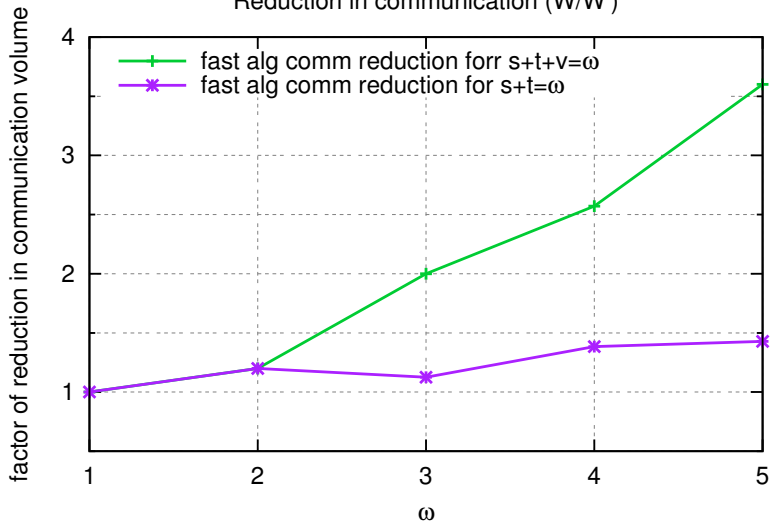
We can lower bound the cost of the fast algorithm using the Hölder-Brascamp-Lieb inequality.

An algorithm that blocks \mathbf{Z} symmetrically nearly attains the cost

$$W'(n, s, t, v, M) = O\left(\frac{\binom{n}{\omega}}{M^{\omega/(\omega - \min(s, t, v))}} \cdot \left[\binom{\omega}{t} + \binom{\omega}{s} + \binom{\omega}{v} \right] + \binom{n}{s+v} + \binom{n}{t+v} + \binom{n}{s+t}\right).$$

which is not far from the lower bound and attains it when $s = t = v$.

Reduction in communication (W/W')



Further communication lower bounds

We can use bilinear algorithm formulations to derive comm. lower bounds

- symmetry preserving tensor contraction algorithms have arbitrary order projections from order d set
- bilinear algorithms¹ provide a more general framework
- a bilinear algorithm is defined by matrices $F^{(A)}$, $F^{(B)}$, $F^{(C)}$,

$$c = F^{(C)}[(F^{(A)T} a) \circ (F^{(B)T} b)]$$

where \circ is the Hadamard (pointwise) product

$$\begin{bmatrix} c \end{bmatrix} = \begin{bmatrix} x & & x & & x & & x \\ x & x & & x & x & & x \\ x & & x & & x & & x \\ x & x & x & & x & x & x \\ x & & x & & x & & x \\ x & x & & x & x & & x \\ x & & x & & x & & x \\ x & x & x & x & x & x & x \end{bmatrix} \left[\left(\begin{bmatrix} x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \end{bmatrix}^T \begin{bmatrix} a \end{bmatrix} \right) \circ \left(\begin{bmatrix} x & x & x & x & x & x & x \\ x & & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & & x & x & x & x & x \\ x & x & x & x & x & x & x \\ x & x & x & x & x & x & x \end{bmatrix}^T \begin{bmatrix} b \end{bmatrix} \right) \right]$$

- communication lower bounds derived based on matrix rank²

¹Pan, Springer, 1984

²S., Hoefler, Demmel, in preparation

Communication cost of symmetry preserving algorithms

For contraction of order $s + v$ tensor with order $v + t$ tensor³

- symmetry preserving algorithm requires $\frac{(s+v+t)!}{s!v!t!}$ fewer multiplies
- matrix-vector-like algorithms ($\min(s, v, t) = 0$)
 - vertical communication dominated by largest tensor
 - horizontal communication asymptotically greater if only unique elements are stored and $s \neq v \neq t$
- matrix-matrix-like algorithms ($\min(s, v, t) > 0$)
 - vertical and horizontal communication costs asymptotically greater for symmetry preserving algorithm when $s \neq v \neq t$

³S., Hoefler, Demmel; Technical Report, ETH Zurich, 2015.

Summary of results

The following table lists the leading order number of multiplications F required by the standard algorithm and F' by the fast algorithm for various cases of symmetric tensor contractions,

| ω | s | t | v | F | F' | applications |
|----------|-----|-----|-----|--|---------------------|----------------------------------|
| 2 | 1 | 1 | 0 | n^2 | $n^2/2$ | syr2, syr2k, her2, her2k |
| 2 | 1 | 0 | 1 | n^2 | $n^2/2$ | symv, symm, hemv, hemm |
| 3 | 1 | 1 | 1 | n^3 | $n^3/6$ | symmetrized matmul |
| $s+t+v$ | s | t | v | $\binom{n}{s} \binom{n}{t} \binom{n}{v}$ | $\binom{n}{\omega}$ | any symmetric tensor contraction |

High-level conclusions:

- The fast symmetric contraction algorithms provide interesting potential arithmetic cost improvements for complex BLAS routines and partially symmetric tensor contractions.
- However, the new algorithms require more communication per flop, incur more numerical error, and usually unable to exploit fused-multiply-add units or blocked matrix multiplication primitives.

Collaborators on various parts:

- James Demmel
- Torsten Hoefler
- Devin Matthews

S., Demmel; Technical Report, ETH Zurich, 2015.

The fast algorithm for computing \mathbf{C} forms the following intermediates with $\binom{n}{\omega}$ multiplications (where $\omega = s + t + v$),

$$Z_i = \left(\sum_{j \in \chi(i)} A_j \right) \cdot \left(\sum_{l \in \chi(i)} B_l \right)$$

$$V_i = \left(\sum_{j \in \chi(i)} A_j \right) \cdot \left(\sum_{k_1} \sum_{l \in \chi(i \cup k)} B_l \right) \\ + \left(\sum_{k_1} \sum_{j \in \chi(i \cup k)} A_j \right) \cdot \left(\sum_{l \in \chi(i)} B_l \right)$$

$$W_i = \left(\sum_{j \in \chi(i)} A_j \right) \cdot \left(\sum_{l \in \chi(i)} B_l \right)$$

$$C_i = \sum_k Z_{i \cup k} - \sum_k V_{i \cup k} \\ - \sum_{j \in \chi(i)} \left(\sum_k W_{j \cup k} \right)$$