Fast and stable matrix multiplication

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joint work James Demmel, Ioana Dumitriu and Robert Kleinberg

The quest for speed

How fast can one multiply two $n \times n$ matrices?

- Standard multiplication: $O(n^3)$ operations.
- Strassen's algorithm: $O(n^{2.81})$ operations.
- ...
- Coppersmith and Winograd's algorithm: $O(n^{2.38})$ operations.
- Is $O(n^2)$ achievable?

Why should we care?

Complexity of matrix multiplication = complexity of "almost all" matrix problems:

- solving linear systems,
- evaluating determinants,
- LU factorization,
- many more.

See P. Bürgisser, M. Clausen, M. A. Shokrollahi Algebraic complexity theory.

Strassen's algorithm

Volker Strassen

Gaussian elimination is not optimal. **Numer. Mathematik [1969].**

Main idea:

- Multiplication by recursively partitioning into smaller blocks.
- To be faster than $O(n^3)$, this needs a method to multiply small matrices (order k) using $o(k^3)$ multiplications.

Strassen

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \times \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix}$$

requires only 7 multiplications:

$$\begin{aligned}
M_1 &:= (A_{11} + A_{22})(B_{11} + B_{22}) \\
M_2 &:= (A_{21} + A_{22})B_{11} \\
M_3 &:= A_{11}(B_{12} - B_{22}) \\
M_4 &:= A_{22}(B_{21} - B_{11}) \\
M_5 &:= (A_{11} + A_{12})B_{22} \\
M_6 &:= (A_{21} - A_{11})(B_{11} + B_{12}) \\
M_7 &:= (A_{12} - A_{22})(B_{21} + B_{22}).
\end{aligned}$$

Strassen

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

where $$\begin{aligned} C_{11} &:= M_1 + M_4 - M_5 + M_7 \\ C_{12} &:= M_3 + M_5 \\ C_{21} &:= M_2 + M_4 \\ C_{22} &:= M_1 - M_2 + M_3 + M_6. \end{aligned}$$

Applied recursively, this yields running time $O(n^{\log_2 7}) \approx O(n^{2.8})$.

Coppersmith and Winograd

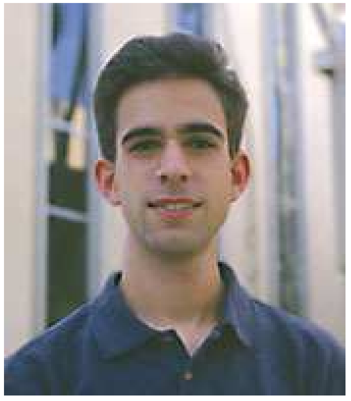
Don Coppersmith

Shmuel Winograd

Matrix multiplication via arithmetic progressions. **Journal of Symbolic Computation [1990].**

Used a thm on dense sets of integers containing no three terms in arithmetic progression (R. Salem & D. C. Spencer [1942]) to get an algorithm with running time $\approx O(n^{2.376})$.

Group-theoretic approach



Chris Umans

Henry Cohn

A group-theoretic approach to matrix multiplication, **FOCS Proceedings [2003].**

Proposed embedding into group algebra to be combined with recursive partitioning.

Why group algebras?

Multiplying two polynomials has complexity $O(n \log n)$ instead of $O(n^2)$ by embedding coefficients into $\mathbb{C}[G]$ where G is a finite cyclic group of order $N \geq 2n$, via the map

$$p \mapsto \{p(w) : w = \exp(2\pi k\mathrm{i}/N)\}_{k=0,\ldots,N-1}.$$

$$\boxed{\begin{array}{l}\text{embed}\\ \text{into } \mathbb{C}[G]\end{array}} \longrightarrow \boxed{\begin{array}{l}\text{convolve}\\ \text{using FFT}\end{array}} \longrightarrow \boxed{\begin{array}{l}\text{extract}\\ \text{from } \mathbb{C}[G]\end{array}}.$$

The same can be done with matrix products, via the map $A \mapsto \sum_{x,y} A(x,y)x^{-1}y$. The group G must have special properties.

The algorithm

- Embed A, B in group algebra
- Perform FFT
- Reorganize results into new matrices
- Multiply new matrices recursively
- Reorganize results into new matrices
- Perform Inverse FFT
- Extract $C = AB$ from group algebra

Properties required

- For unambiguous embedding into $\mathbb{C}[G]$ there must be three subgroups H_1, H_2, H_3 with the triple product property :

  $$h_1 h_2 h_3 = 1, h_i \in H_i \implies h_1 = h_2 = h_3 = 1$$

  (can be generalized to other subsets of G).
- For the resulting algorithm to be faster than $O(n^3)$, we must beat the sum of the cubes:

  $$|H_1|\,|H_2|\,|H_3| > \sum_j d_j^3$$

  (d_j are the character degrees of G).

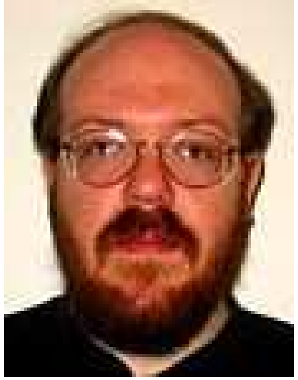
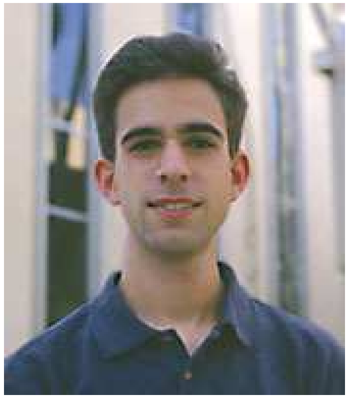
Wedderburn's theorem

Theorem. The group algebra of a finite group G decomposes as the direct product

$$\mathbb{C}[G] \cong \mathbb{C}^{d_1 \times d_1} \times \cdots \times \mathbb{C}^{d_k \times d_k}$$

of matrix algebras of orders $d_1, \ldots, d_k$. These orders are the character degrees of G, or the dimensions of its irreducible representations.

Beating the sum of the cubes

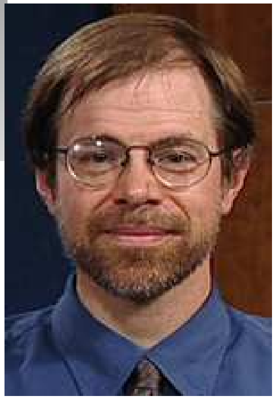

Balázs Szegedy   Henry Cohn   Chris Umans   Bobby Kleinberg

Group-theoretic algorithms for matrix multiplication,
FOCS Proceedings [2005].

Found groups with subsets beating the sum of the cubes and satisfying the triple product property.

Press coverage: *SIAM News [Nov 2005]* by Sara Robinson.

Error analysis



Jim Demmel

Ioana Dumitriu

Olga Holtz

Bobby Kleinberg

Fast matrix multiplication is stable, **ArXiv Math.NA/0603207 [2006].**

Main question: Do you get the right answer in the presence of roundoff? To answer, need error analysis for a large class of recursive matrix multiplication algorithms.

Method

Forward error analysis in the spirit of

D. Bini and G. Lotti ***Stability of fast algorithms for matrix multiplication,*** **Numer. Mathematik [1980/81]**.

What was missing:

- More general roundoff assumptions
- Wider scope:

  nonstationary algorithms

  algorithms with pre- and post- processing

Recursive matmul algorithms

aka Bilinear noncommutative algorithms

- *Stationary partitioning* algorithms: at each step, split matrices into the same number k^2 of square blocks.
- *Non-stationary partitioning* algorithms: the number of blocks may vary at each step.
- Partitioning may be combined with *pre- and post-processing*, both linear maps that introduce roundoff errors.

Error bounds

In all cases, the error bounds have the form

$$\|C_{comp} - C\| \le cn^d \varepsilon \|A\| \cdot \|B\| + O(\varepsilon^2),$$

where	c, d	are	modest constants,
	ε		machine precision,
	n		order of A, B, $C = AB$,
	C_{comp}		computed value of C.

Cf. with error bound for n^3-algorithm:

$$|C_{comp} - C| \le cn\varepsilon |A| \cdot |B| + O(\varepsilon^2).$$

Group-theoretic algorithms

- Embed A, B in group algebra (exact)
- Perform FFT (roundoff)
- Reorganize results into new matrices (exact)
- Multiply new matrices recursively (roundoff)
- Reorganize results into new matrices (exact)
- Perform Inverse FFT (roundoff)
- Extract $C = AB$ from group algebra (exact)

Semi-direct product, wreath product

If H is any group and Q is a group which acts (on the left) by automorphisms of H, with $q \cdot h$ denoting the action of $q \in Q$ on $h \in H$, then the semidirect product $H \rtimes Q$ is the set of ordered pairs (h, q) with the multiplication law

$$(h_1, q_1)(h_2, q_2) = (h_1(q_1 \cdot h_2), q_1 q_2).$$

If H is any group, S is any finite set, and Q is a group with a left action on S, the wreath product $H \wr Q$ is the semidirect product $(H^S) \rtimes Q$ where Q acts on the direct product of $|S|$ copies of H by permuting the coordinates according to the action of Q on S.

Running example, I

Consider the set $S = \{0, 1\}$ and a two-element group Q whose non-identity element acts on S by swapping 0 and 1. Let H be the group $(\mathbb{Z}/16)^3$. An element of H^S is an ordered pair of elements of H:

$$\begin{pmatrix} x_{00} & x_{01} & x_{02} \\ x_{10} & x_{11} & x_{12} \end{pmatrix}.$$

An element of $H \wr Q$ is an ordered pair (X, q) where X is a matrix as above, and $q = \pm 1$. Example:

$$\begin{array}{c} (X, -1) \\ \cdot (Y, -1) \end{array} = \left(\begin{pmatrix} x_{00} + y_{10} & x_{01} + y_{11} & x_{02} + y_{12} \\ x_{10} + y_{00} & x_{11} + y_{01} & x_{12} + y_{02} \end{pmatrix}, 1 \right)$$

Triple product property

If S, T are subsets of a group G, let $Q(S, T)$ denote their right quotient set:

$$\begin{aligned} Q(S,T) &:= \{st^{-1} : s \in S, t \in T\}, \\ Q(S) &:= Q(S,S). \end{aligned}$$

Definition. If H is a group and X, Y, Z are three subsets, we say X, Y, Z satisfy the triple product property if, for all $q_x \in Q(X)$, $q_y \in Q(Y)$, $q_z \in Q(Z)$, the condition $q_x q_y q_z = 1$ implies $q_x = q_y = q_z = 1$.

Simultaneous triple product property

If $\{(X_i, Y_i, Z_i) : i \in I\}$ is a collection of ordered triples of subsets of H, we say that this collection satisfies the simultaneous triple product property (STPP) if, for all $i, j, k \in I$ and all $q_x \in Q(X_i, X_j)$, $q_y \in Q(Y_j, Y_k)$, $q_z \in Q(Z_k, Z_i)$, the condition $q_x q_y q_z = 1$ implies $q_x{=}q_y{=}q_z{=}1$ and $i{=}j{=}k$.

Lemma If a group H has subsets $\{X_i, Y_i, Z_i\}_{1 \le i \le n}$ satisfying the simultaneous triple product property, then for every element $h\pi$ in $H \wr \mathrm{Sym}_n$ there is at most one way to represent $h\pi$ as a quotient $(x\sigma)^{-1} y\tau$ such that $x \in \prod_{i=1}^{n} X_i$, $y \in \prod_{i=1}^{n} Y_i$, $\sigma, \tau \in \mathrm{Sym}_n$.

Running example, II

In our running example, the group H is $(\mathbb{Z}/16\mathbb{Z})^3$. Consider the following three subgroups of H.

$$\begin{aligned} X &:= (\mathbb{Z}/16\mathbb{Z}) \times \{0\} \times \{0\} \\ Y &:= \{0\} \times (\mathbb{Z}/16\mathbb{Z}) \times \{0\} \\ Z &:= \{0\} \times \{0\} \times (\mathbb{Z}/16\mathbb{Z}) \end{aligned}$$

Then X, Y, Z satisfy the triple product property: if $q_x \in Q(X), q_y \in Q(Y), q_z \in Q(Z)$, and $q_x + q_y + q_z = 0$, then $q_x = q_y = q_z = 0$.

Running example, IIa

Now consider the following six subsets of H:

$$\begin{aligned}
\overline{X}_0 &:= \{1,2,\ldots,15\} \times \{0\} \times \{0\} \\
\overline{Y}_0 &:= \{0\} \times \{1,2,\ldots,15\} \times \{0\} \\
\overline{Z}_0 &:= \{0\} \times \{0\} \times \{1,2,\ldots,15\} \\
\overline{X}_1 &:= \{0\} \times \{1,2,\ldots,15\} \times \{0\} \\
\overline{Y}_1 &:= \{0\} \times \{0\} \times \{1,2,\ldots,15\} \\
\overline{Z}_1 &:= \{1,2,\ldots,15\} \times \{0\} \times \{0\}.
\end{aligned}$$

Then $(\overline{X}_0, \overline{Y}_0, \overline{Z}_0)$ and $(\overline{X}_1, \overline{Y}_1, \overline{Z}_1)$ satisfy the simultaneous triple product property.

Discrete Fourier transform

If H is an abelian group, let $\widehat{H}$ denote the set of all homomorphisms from H to S^1 aka characters. Canonical bijection $(\chi_1, \chi_2) \mapsto \chi$:

$$\chi(h_1, h_2) = \chi_1(h_1)\chi_2(h_2).$$

There is a left action of Sym_n on the set $\widehat{H}^n$:

$$\sigma \cdot (\chi_1, \chi_2, \ldots, \chi_n) := (\chi_{\sigma^{-1}(1)}, \chi_{\sigma^{-1}(2)}, \ldots, \chi_{\sigma^{-1}(n)}).$$

Denote by $\Xi(H^n)$ a subset of $\widehat{H}^n$ containing exactly one representative of each orbit of the Sym_n action on $\widehat{H}^n$. Note $|\Xi(H^n)| = \binom{|H|+n-1}{n}$.

Running example, III

A character χ of the group $H = (\mathbb{Z}/16\mathbb{Z})^3$ is uniquely determined by a triple (a_1, a_2, a_3) of integers modulo 16. For an element $h = (b_1, b_2, b_3) \in H$,

$$\chi(h) = e^{2\pi i(a_1 b_1 + a_2 b_2 + a_3 b_3)/16}.$$

A character of the group H^2 may be represented as

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix}$$

as before. The group $\mathrm{Sym}_2 = \{\pm 1\}$ acts on $\widehat{H^2}$ by exchanging the two rows of such a matrix. The set $\Xi(H^2)$ has cardinality $\binom{4096}{2} + 4096 = 8{,}390{,}656.$

Abelian STP families

An abelian STP family with growth parameters (α, β) is a collection of ordered triples (H_N, Υ_N, k_N), satisfying

1. H_N is an abelian group.
2. $\Upsilon_N = \{(X_i, Y_i, Z_i) : i = 1, 2, \ldots, N\}$ is a collection of N ordered triples of subsets of H_N satisfying the simultaneous triple product property.
3. $|H_N| = N^{\alpha + o(1)}$.
4. $k_N = \prod_{i=1}^{N} |X_i| = \prod_{i=1}^{N} |Y_i| = \prod_{i=1}^{N} |Z_i| = N^{\beta N + o(N)}$.

Remark

If $\{(H_N, \Upsilon_N, k_N)\}$ is an abelian STP family, then Lemma above ensures that there is a 1-1 mapping

$$\left(\prod_{i=1}^{N} X_i\right) \times \left(\prod_{i=1}^{N} Y_i\right) \times (\mathrm{Sym}_N)^2 \longrightarrow H_N \wr \mathrm{Sym}_N$$

given by $(x, y, \sigma, \tau) \mapsto (x\sigma)^{-1} y\tau$. This implies also

$$\begin{aligned} |H_N|^N N! &\geq (k_N N!)^2 \\ N^{\alpha N + o(N)} N^{N + o(N)} &\geq N^{2\beta N + o(N)} N^{2N + o(N)} \\ \alpha + 1 &\geq 2\beta + 2 \\ \frac{\alpha - 1}{\beta} &\geq \frac{\alpha + 1}{\beta + 1} \geq 2. \end{aligned}$$

Running example, IV

Extend our example to an abelian STP family. For $N \geq 1$ let $\ell = \lceil \log_2(N) \rceil$ and let $H_N = H^\ell$. For $1 \leq i \leq N$ let $i_1, i_2, \ldots, i_\ell$ denote the binary digits of the number $i - 1$ (padded with initial 0's so that it has exactly ℓ digits) and let

$$X_i = \prod_{m=1}^{\ell} \bar{X}_{i_m}, \quad Y_i = \prod_{m=1}^{\ell} \bar{Y}_{i_m}, \quad Z_i = \prod_{m=1}^{\ell} \bar{Z}_{i_m}.$$

The triples (X_i, Y_i, Z_i) satisfy the simultaneous triple product property.

Running example, IV

Growth parameters of this abelian STP family.

$|H_N| = |H|^{\ell} = (16^3)^{1+\lfloor \log_2(N) \rfloor} = N^{3\log_2(16)+O(1/\log N)}$,

hence $\alpha = 3\log_2(16) = 12$. Also,

$$\begin{aligned} k_N &= \prod_{i=1}^{N} |X_i| = \prod_{i=1}^{N} \prod_{m=1}^{\ell} |\bar{X}_{i_m}| = 15^{N\ell} \\ &= 15^{N\log_2(N)+O(N)} = N^{N\log_2(15)+O(N/\log N)}, \end{aligned}$$

hence $\beta = \log_2(15)$.

Abelian STP algorithms

- The non-abelian group used in the algorithm is a wreath product of H_N with the symmetric group S_N.
- The mapping from $\mathbb{C}[G]$ to a product of matrix algebras, in the Wedderburn thm, is computed by applying $N!$ copies of FFT of H_N, in parallel.
- The three subsets satisfying the triple product property are defined using the sets X_i, Y_i, Z_i.
- The resulting algorithm has running time $O(n^{(\alpha-1)/\beta+o(1)})$.

Algorithm

- **Embedding** (NO ARITHMETIC): Compute the following pair of vectors in $\mathbb{C}[H \wr \mathrm{Sym}_N]$.

$$
\begin{aligned}
a &= \sum_{x \in X} \sum_{y \in Y} A_{xy} \mathrm{e}_{x^{-1}y} \\
b &= \sum_{y \in Y} \sum_{z \in Z} B_{yz} \mathrm{e}_{y^{-1}z}.
\end{aligned}
$$

- **Fourier transform** (ARITHMETIC): Compute the following pair of vectors in $\mathbb{C}[\widehat{H}^N \rtimes \mathrm{Sym}_N]$.

$$\hat{a} = \sum_{\chi \in \widehat{H}^N} \sum_{\sigma \in \mathrm{Sym}_N} \left(\sum_{h \in H^N} \chi(h) a_{\sigma h} \right) \mathrm{e}_{\chi,\sigma}.$$

$$\hat{b} = \sum_{\chi \in \widehat{H}^N} \sum_{\sigma \in \mathrm{Sym}_N} \left(\sum_{h \in H^N} \chi(h) b_{\sigma h} \right) \mathrm{e}_{\chi,\sigma}.$$

Algorithm

- **Assemble matrices** (NO ARITHMETIC): For every $\chi \in \Xi(H^N)$, compute the following pair of matrices A^χ, B^χ, whose rows and columns are indexed by elements of Sym_N.

$$
\begin{aligned}
A^\chi_{\rho\sigma} &= \hat{a}_{\rho\cdot\chi,\sigma\rho^{-1}} \\
B^\chi_{\sigma\tau} &= \hat{b}_{\sigma\cdot\chi,\tau\sigma^{-1}}
\end{aligned}
$$

Algorithm

- **Multiply matrices** (ARITHMETIC): For every $\chi \in \Xi(H^N)$, compute the matrix product $C^\chi = A^\chi B^\chi$ by recursively applying the abelian STP algorithm.

- **Disassemble matrices** (NO ARITHMETIC):
Compute a vector
$\hat{c} = \sum_{\chi,\sigma} \hat{c}_{\chi,\sigma} e_{\chi,\sigma} \in \mathbb{C}[\widehat{H}^N \rtimes \mathrm{Sym}_N]$ whose components $\hat{c}_{\chi,\sigma}$ are defined as follows.
Given χ, σ, let $\chi_0 \in \Xi(H^N)$ and $\tau \in \mathrm{Sym}_N$ be such that $\chi = \tau \cdot \chi_0$. Let

$$\hat{c}_{\chi,\sigma} := C^{\chi_0}_{\tau,\sigma\tau}.$$

- **Inverse Fourier transform** (ARITHMETIC): Compute the following vector $c \in \mathbb{C}[H \wr \mathrm{Sym}_N]$.

$$c = \sum_{h \in H^N} \sum_{\sigma \in \mathrm{Sym}_N} \left(\frac{1}{|H|^N} \sum_{\chi \in \widehat{H}^N} \chi(-h) \hat{c}_{\chi,\sigma} \right) \mathrm{e}_{\sigma h}.$$

- **Output** (NO ARITHMETIC): Output the matrix $C = (C_{xz})$ whose entries are given by the formula

$$C_{xz} = c_{x^{-1}z}.$$

Running example, V

In our example with $H = (\mathbb{Z}/16\mathbb{Z})^3$ and $N = 2$, we have $k_N N! = (15^2)(2!) = 450$, so the seven steps above constitute a reduction from 450-by-450 matrix multiplication to $|\Xi(H^2)|$ 2-by-2 matrix multiplication problems. Recall that $|\Xi(H^2)| = 8{,}390{,}656$.

By comparison, the naive reduction from 450-by-450 to 2-by-2 matrix multiplication — by partitioning each matrix into $(225)^2$ square blocks of size 2-by-2 — would require the algorithm to compute $(225)^3 = 11{,}390{,}625$ smaller matrix products.

Using this for recurrence gives running time $O(n^{2.95})$.

Running example, V

Instead, if we use the $N = 2, H = (\mathbb{Z}/16\mathbb{Z})^3$ construction as the basis of an abelian STP family, we may apply the abelian STP algorithm which uses a more sophisticated recursion as the size of the matrices grows to infinity. For example, when $N = 2^\ell$, we have $n = k_N N! = 15^{N\ell}(2^\ell)!$. matrix multiplications. As $N! = O(n^{0.21})$, the resulting running time can be shown to be $O(n^{2.81})$.

Theorem. If $\{(H_N, \Upsilon_N, k_N)\}$ is an abelian STP family with growth parameters (α, β), then the corresponding abelian STP algorithm is stable. It satisfies the error bound

$$\|C_{comp} - C\|_F \leq \mu(n)\varepsilon\|A\|_F \cdot \|B\|_F + O(\varepsilon^2),$$

with the Frobenius norm $\|\cdot\|_F$ and the function μ of order

$$\mu(n) = n^{\frac{\alpha+2}{2\beta} + o(1)}.$$

Highlight II

Let ω be the exponent of matrix multiplication.

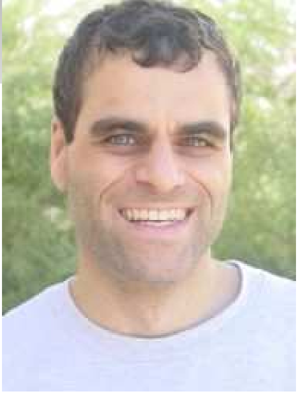
Theorem. For every $\alpha > 0$ there exists an algorithm for multiplying $n \times n$ matrices that performs $O(n^{\omega+\alpha})$ operations and satisfies the bound

$$\|C_{comp} - C\| \leq \mu(n)\varepsilon\|A\| \cdot \|B\| + O(\varepsilon^2),$$

with $\mu(n) = O(n^c)$ for some constant c that depends on α but not on n.

Remark: It is an open question whether a group-theoretic algorithm can achieve $O(n^{\omega+\alpha})$ for arbitrarily small α.

Result used



Ran Raz

On the complexity of matrix product

SIAM J. Computing [2003].

Theorem. The exponent of matrix multiplication is achievable by bilinear noncommutative algorithms. More precisely, for every arithmetic circuit of size S which computes the product of two matrices A, B over a field with characteristic zero, there is a bilinear circuit of size $O(S)$ that also computes the product of A and B.

Tradeoff between n and ε

All our bounds are of the form

$$\|C_{comp} - C\| \le \mu(n)\varepsilon\|A\| \cdot \|B\| + O(\varepsilon^2), \quad (*)$$

$\mu(n) = O(n^c)$ for some constant $c \ge 1$.

As $\mu(n)\varepsilon \ll 1$, the number b of bits to represent fractional part of floating point numbers satisfies $b = \log_2(1/\varepsilon) \ge \log_2 n$.

Multiplying the number of bits by a factor f raises the cost of an algorithm by $O(f^{1+o(1)})$ using Schönhage-Strassen [1971].

All algorithms satisfying $(*)$ are in fact $O(\cdot)$-equivalent.

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Fast matrix multiplication is stable

Authors: James Demmel, Ioana Dumitriu, Olga Holtz, Robert Kleinberg
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MSC-class: 65Y20, 65F30, 65G50, 68Q17, 68W40, 20C05, 20K01, 16S34, 43A30, 65T50

We perform forward error analysis for a large class of recursive matrix multiplication algorithms in the spirit of [D. Bini and G. Lotti, Stability of fast algorithms for matrix multiplication, Numer. Math. 36 (1980), 63--72]. As a consequence of our analysis, we show that the exponent of matrix multiplication can be achieved by numerically stable algorithms. We also show that new group-theoretic algorithms proposed in [H. Cohn, and C. Umans, A group-theoretic approach to fast matrix multiplication, FOCS 2003, 438--449] and [H. Cohn, R. Kleinberg, B. Szegedy and C. Umans, Group-theoretic algorithms for matrix multiplication, FOCS 2005, 379--388] are all included in the class of algorithms to which our analysis applies, and are therefore numerically stable. We perform detailed error analysis for three specific fast group-theoretic algorithms.

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