Fast and stable matrix multiplication

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joint work James Demmel, Ioana Dumitriu and Robert Kleinberg

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• Standard multiplication: $O(n^3)$ operations.

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- 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.

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

Strassen's algorithm



Volker Strassen

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

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

$$\left[egin{array}{cccc} A_{11} & A_{12} \ A_{21} & A_{22} \end{array}
ight] imes \left[egin{array}{cccc} B_{11} & B_{12} \ B_{21} & B_{22} \end{array}
ight] & ext{requires only} \ 7 & ext{multiplications:} \ M_1 &:= & (A_{11} + A_{22})(B_{11} + B_{22}) \ M_2 &:= & (A_{21} + A_{22})B_{11} \ M_3 &:= & A_{11}(B_{12} - B_{22}) \ M_4 &:= & A_{22}(B_{21} - B_{11}) \ M_5 &:= & (A_{11} + A_{12})B_{22} \ M_6 &:= & (A_{21} - A_{11})(B_{11} + B_{12}) \ M_7 &:= & (A_{12} - A_{22})(B_{21} + B_{22}). \end{array}$$

Strassen

Then
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 where $C_{11} := M_1 + M_4 - M_5 + M_7$ $C_{12} := M_3 + M_5$ $C_{21} := M_2 + M_4$ $C_{22} := M_1 - M_2 + M_3 + M_6.$

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 $C_{12} := M_3 + M_5$ $C_{21} := M_2 + M_4$ $C_{22} := M_1 - M_2 + M_3 + M_6.$

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].

Coppersmith and Winograd







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].

Group-theoretic approach



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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

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

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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.

• Embed A, B in group algebra

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- 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 :

 $h_1h_2h_3=1, h_i\in H_i \implies h_1=h_2=h_3=1$ (can be generalized to other subsets of G).

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 (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_i) are the character degrees of G).

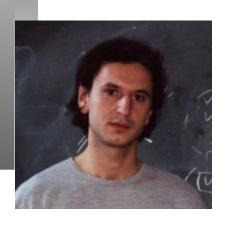
Wedderburn's theorem

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







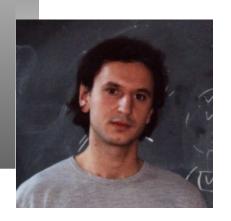


Balázs Szegedy Henry Cohn Chris Umans

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

Beating the sum of the cubes









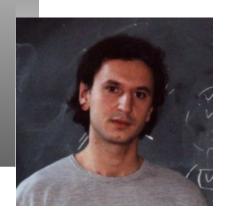
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Found groups with subsets beating the sum of the cubes and satisfying the triple product property.

Beating the sum of the cubes









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

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

Error analysis









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

Error analysis









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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].

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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.

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Recursive matmul algorithms

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- 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, machine precision, order of A,B,C=AB, C_{comp} computed value of C.

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

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

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- 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

$$(h_1,q_1)(h_2,q_2)=(h_1(q_1\cdot h_2),q_1q_2).$$

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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:

$$\left(egin{array}{ccc} x_{00} & x_{01} & x_{02} \ x_{10} & x_{11} & x_{12} \end{array}
ight)$$
 .

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

$$egin{array}{ll} (X,-1) \ \cdot (Y,-1) \end{array} = \left(\left(egin{array}{ccc} x_{00} + y_{10} & x_{01} + y_{11} & x_{02} + y_{12} \ x_{10} + y_{00} & x_{11} + y_{01} & x_{12} + y_{02} \end{array}
ight), 1
ight)$$

Triple product property

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

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

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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 $q_xq_yq_z=1$ implies $q_x=q_y=q_z=1$ and i=j=k.

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Lemma If a group H has subsets $\{X_i,Y_i,Z_i\}_{1\leq i\leq n}$ 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.

$$egin{array}{lll} X &:= & ({\mathbb Z}/16{\mathbb Z}) imes \{0\} imes \{0\} \ Y &:= & \{0\} imes ({\mathbb Z}/16{\mathbb Z}) imes \{0\} \ Z &:= & \{0\} imes \{0\} imes ({\mathbb Z}/16{\mathbb Z}) \ \end{array}$$

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, Ila

Now consider the following six subsets of H:

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 :

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

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 $h=(b_1,b_2,b_3)\in H$,

$$\chi(h) = e^{2\pi i (a_1b_1 + a_2b_2 + a_3b_3)/16}.$$

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

$$\left(egin{array}{ccc} a_{11} & a_{12} & a_{13} \ a_{21} & a_{22} & a_{23} \end{array}
ight)$$

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. $\Upsilon_N = \{(X_i, Y_i, Z_i) : i = 1, 2, ..., N\}$ 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

$$\left(\prod_{i=1}^N X_i
ight) imes \left(\prod_{i=1}^N Y_i
ight) imes (\mathrm{Sym}_N)^2 o H_N\wr \mathrm{Sym}_N$$

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

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

$$egin{array}{ll} |H_N|^N N! & \geq \ (k_N N!)^2 \ N^{lpha N + o(N)} N^{N + o(N)} & \geq \ N^{2eta N + o(N)} N^{2N + o(N)} \ lpha + 1 & \geq \ 2eta + 2 \ rac{lpha - 1}{eta} & \geq \ rac{lpha + 1}{eta + 1} & \geq \ 2. \end{array}$$

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_ℓ denote the binary digits of the number i-1 (padded with initial 0's so that it has exactly ℓ digits) and let

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

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,

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

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

Abelian STP algorithms

- The non-abelian group used in the algorithm is a wreath product of ${\cal H}_N$ 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 $O(n^{(\alpha-1)/\beta+o(1)})$.

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

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

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

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

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

• 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 .

$$egin{array}{lll} A_{
ho\sigma}^{\chi} &=& \hat{a}_{
ho\cdot\chi,\sigma
ho^{-1}} \ & \ B_{\sigma au}^{\chi} &=& \hat{b}_{\sigma\cdot\chi, au\sigma^{-1}} \end{array}$$

• 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

 $\hat{c} = \sum_{\chi,\sigma} \hat{c}_{\chi,\sigma} \mathbf{e}_{\chi,\sigma} \in \mathbb{C}[\widehat{H}^N
times \mathrm{Sym}_N]$ 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

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

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

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

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• 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

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

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

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

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

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

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

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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 \boldsymbol{A} , \boldsymbol{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.

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 $c \geq 1$.

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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].

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

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[math/0603207] Fast matrix multiplication is stable

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Fast matrix multiplication is stable

Authors: James Demmel, Ioana Dumitriu, Olga Holtz, Robert Kleinberg

Comments: 14 pages

Subj-class: Numerical Analysis; Group Theory; Computational Complexity; Data Structures and Algorithms 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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