# Accurate and efficient expression evaluation and linear algebra 

James Demmel<br>UC Berkeley<br>Math and EECS Depts.

Joint work with
Ioana Dumitriu, Olga Holtz, Plamen Koev

## Topics.

1. Getting the right answer

- At all? In polynomial time?
- Depends on the model of arithmetic


## Topics.

1. Getting the right answer

- At all? In polynomial time?
- Depends on the model of arithmetic

2. Getting the same answer

- When running same problem on two different machines?
- When running same problem twice on same machine?


## Topics.

1. Getting the right answer

- At all? In polynomial time?
- Depends on the model of arithmetic

2. Getting the same answer

- When running same problem on two different machines?
- When running same problem twice on same machine?

3. Getting a fast answer

- Arithmetic is cheap, moving data is expensive
- How does this change algorithms?


## Topics.

1. Getting the right answer

- At all? In polynomial time?
- Depends on the model of arithmetic

2. Getting the same answer

- When running same problem on two different machines?
- When running same problem twice on same machine?

3. Getting a fast answer

- Arithmetic is cheap, moving data is expensive
- How does this change algorithms?


## Motivating Example (1/2)

Def: Accurate means relative error less than 1
How do the following 3 kinds of accurate evaluation problems differ in difficulty?

1. Motzkin polynomial $z^{6}+x^{2} y^{2}\left(x^{2}+y^{2}-3 z^{2}\right)$, or $\operatorname{eig}(V)$ with $V_{i j}=x_{i}^{j}$, where $0<x_{1}<x_{2}<\ldots$
2. Eigenvalues of $\nabla \cdot(\theta \nabla u)+\lambda \rho u=0$ discretized with the FEM on a triangular mesh, or $x+y+z$
3. Determinant of a Toeplitz matrix

## Motivating Example (2/2)

Accurate alg. for Motzkin polynomial $p=z^{6}+x^{2} y^{2}\left(x^{2}+y^{2}-3 z^{2}\right)$

$$
\text { if } \begin{aligned}
& |x-z| \leq|x+z| \wedge|y-z| \leq|y+z| \\
p= & z^{4} \cdot\left[4\left((x-z)^{2}+(y-z)^{2}+(x-z)(y-z)\right)\right]+ \\
& +z^{3} \cdot\left[2 \left(2(x-z)^{3}+5(y-z)(x-z)^{2}+5(y-z)^{2}(x-z)+\right.\right. \\
& \left.\left.2(y-z)^{3}\right)\right]+ \\
+ & z^{2} \cdot\left[(x-z)^{4}+8(y-z)(x-z)^{3}+9(y-z)^{2}(x-z)^{2}+\right. \\
& \left.8(y-z)^{3}(x-z)+(y-z)^{4}\right]+ \\
+ & z \cdot\left[2 ( y - z ) ( x - z ) \left((x-z)^{3}+2(y-z)(x-z)^{2}+\right.\right. \\
& \left.2(y-z)^{2}(x-z)+(y-z)^{3}\right]+ \\
& +(y-z)^{2}(x-z)^{2}\left((x-z)^{2}+(y-z)^{2}\right)
\end{aligned}
$$

else ... 7 more analogous cases

Can we automate the discovery of such algorithms? Or prove they do not exist, i.e. that extra precision is necessary? How much extra precision?

## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Problem statement

Given a polynomial (or a family of polynomials) $p$, either produce an accurate algorithm to compute $y=p(x)$, or prove that none exists.

Accurately means relative error $\eta<1$, i.e.
$\diamond\left|y_{\text {computed }}-y\right| \leq \eta|y|$,
$\diamond \eta=10^{-2}$ yields two digits of accuracy,
$\diamond y_{\text {computed }}=0 \Longleftrightarrow y=0$.

50x50 Hilbert Matrix $-\log _{10}$ (eigenvalues)


$$
H_{i j}=1 /(i+j-1)
$$

## 40x40 Pascal Matrix - eigenvalues



20x20 Schur Complement of 40x40 Vandermonde Matrix - eigenvalues


## Complexity of Accurate Algorithms for General Structured Matrices

| Type of matrix | $\operatorname{det} A$ | $A^{-1}$ | Any <br> minor | LDU | SVD | Sym <br> EVD |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| Acyclic <br> (bidiagonal and other) | $n$ | $n^{2}$ | $n$ | $\leq n^{2}$ | $n^{3}$ | N/A |
| Total Sign Compound <br> (TSC) | $n$ | $n^{3}$ | $n$ | $n^{4}$ | $n^{4}$ | $n^{4}$ |
| Diagonally Scaled Totally <br> Unimodular (DSTU) | $n^{3}$ | $n^{5} ?$ | $n^{3}$ | $n^{3}$ | $n^{3}$ | $n^{3}$ |
| Weakly diagonally <br> dominant M-matrix | $n^{3}$ | $n^{3}$ | $?$ | $n^{3}$ | $n^{3}$ | $n^{3}$ |
| Displace- Cauchy <br> ment Vandermonde <br> Rank One | $n^{2}$ | $n^{2}$ | $n^{2}$ | $\leq n^{3}$ | $n^{3}$ | $n^{3}$ |
| Polynomial <br> Toeplitz | $n^{2}$ | $?$ | $?$ | $?$ | $n^{3}$ | $n^{3}$ |

Complexity of Accurate Algorithms for Totally Nonnegative (TN) Matrices

| Type of Matrix | $\operatorname{det} A$ | $A^{-1}$ | $\begin{gathered} \text { Any } \\ \text { minor } \end{gathered}$ | Gauss. elim. |  |  | $\begin{aligned} & \text { NE } \\ & \text { NP } \end{aligned}$ | $A x=b$ | SVD | Eig <br> Val. |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Cauchy | $n^{2}$ | $n^{2}$ | $n^{2}$ | $n^{2}$ | $n^{3}$ | $n^{3}$ | $n^{2}$ | $n^{2}$ | $n^{3}$ | $n^{3}$ |
| Vandermonde | $n^{2}$ | $n^{3}$ | $n^{3}$ | $n^{2}$ | $n^{2}$ | poly | $n^{2}$ | $n^{2}$ | $n^{3}$ | $n^{3}$ |
| Generalized Vandermonde | $n^{2}$ | $n^{3}$ | poly | $n^{2}$ | $n^{2}$ | poly | $n^{2}$ | $n^{2}$ | $n^{3}$ | $n^{3}$ |
| Any TN in Neville form | $n$ | $n^{3}$ | $n^{3}$ | $n^{3}$ | $n^{3}$ | $n^{3}$ | 0 | $n^{2}$ | $n^{3}$ | $n^{3}$ |

Def: $A$ is Totally Positive (TP) if all minors are positive. $A$ is Totally Nonnegative (TN) if all minors are nonnegative.

Theorem: The class of TN matrices for which we can do accurate linear algebra in polynomial time is closed under multiplication, taking submatrices, Schur complement, J-inverse and converse.

## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$ $\circ$ Operations?


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$ $\circ$ Operations?
$\diamond$ in Classical Model (CM),,$+-\times$; also exact negation;


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$ - Operations?
$\diamond$ in Classical Model $(\mathrm{CM}),+,-, \times$; also exact negation;
$\diamond$ in Black-Box Model (BBM), in addition to the above, polynomial expressions (e.g. $x-y \cdot z$ (FMA), $x+y+z$, dot products, small determinants, ...)
- Constants?


## Availability of constants?

- Classical Model:
- without $\sqrt{2}$, we cannot compute

$$
x^{2}-2=(x-\sqrt{2})(x+\sqrt{2})
$$

accurately.

- no loss of generality for homogeneous, integer-coefficient polynomials.
- Black-Box Model:
- any constants we choose can be accommodated.


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$
- Operations?
$\diamond$ in Classical Model $(\mathrm{CM}),+,-, \times$; also exact negation;
$\diamond$ in Black-Box Model (BBM), in addition to the above, polynomial expressions (e.g. $x-y \cdot z$ (FMA), $x+y+z$, dot products, small determinants, ...)
- Constants? none in Classical Model, anything in Black-Box Model.


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$
- Operations?
$\diamond$ in Classical Model $(\mathrm{CM}),+,-, \times$ also exact negation;
$\diamond$ in Black-Box Model (BBM), in addition to the above, polynomial expressions (e.g. $x-y \cdot z$ (FMA), $x+y+z$, dot products, small determinants, ...)
- Algorithms?
$\diamond$ exact answer in finite \# of steps in absence of roundoff error


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$
$\circ$ Operations?
$\diamond$ in Classical Model $(\mathrm{CM}),+,-, \times$ also exact negation;
$\diamond$ in Black-Box Model (BBM), in addition to the above, polynomial expressions (e.g. $x-y \cdot z$ (FMA), $x+y+z$, dot products, small determinants, ...)
- Algorithms?
$\diamond$ exact answer in finite \# of steps in absence of roundoff error
$\diamond$ branching based on comparisons


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
- $f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$
- Operations?
$\diamond$ in Classical Model $(\mathrm{CM}),+,-, \times$ also exact negation;
$\diamond$ in Black-Box Model (BBM), in addition to the above, polynomial expressions (e.g. $x-y \cdot z$ (FMA), $x+y+z$, dot products, small determinants, ...)
- Algorithms?
$\diamond$ exact answer in finite \# of steps in absence of roundoff error
$\diamond$ branching based on comparisons
$\diamond$ non-determinism (because determinism is simulable)


## Model(s) of Arithmetic.

- All quantities are arbitrary real numbers, or complex numbers (bits come later)
$\circ f l(a \otimes b)=(a \otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon \ll 1$
- Operations?
$\diamond$ in Classical Model $(\mathrm{CM}),+,-, \times$ also exact negation;
$\diamond$ in Black-Box Model (BBM), in addition to the above, polynomial expressions (e.g. $x-y \cdot z$ (FMA), $x+y+z$, dot products, small determinants, ...)
- Algorithms?
$\diamond$ exact answer in finite \# of steps in absence of roundoff error
$\diamond$ branching based on comparisons
$\diamond$ non-determinism (because determinism is simulable)
$\diamond$ domains to be $\mathbb{C}^{n}$ or $\mathbb{R}^{n}$ (but some domain-specific results).


## Problem Statement, formally:

$\diamond$ Notation:
$-p(x)$ multivariate polynomial to be evaluated, $x=\left(x_{1}, \ldots, x_{k}\right)$.
$-\delta=\left(\delta_{1}, \ldots, \delta_{m}\right)$ is the vector of error (rounding) variables.
$-p_{\text {comp }}(x, \delta)$ is the result of algorithm to compute $p$ at $x$ with errors $\delta$.
$\diamond$ Goal: Decide if $\exists$ algorithm $p_{\text {comp }}(x, \delta)$ to accurately evaluate $p(x)$ on $\mathcal{D}$ :

$$
\begin{aligned}
& \forall 0<\eta<1 \quad \ldots \text { for any } \eta=\text { desired relative error } \\
& \exists 0<\epsilon<1 \quad \ldots \text { there is an } \epsilon=\text { maximum rounding error } \\
& \forall x \in \mathcal{D} \quad \ldots \text { so that for all } x \text { in the domain } \\
& \forall\left|\delta_{i}\right| \leq \epsilon \quad \ldots \text { and for all rounding errors bounded by } \epsilon \\
& \quad\left|p_{\text {comp }}(x, \delta)-p(x)\right| \leq \eta \cdot|p(x)| \ldots \text { relative error is at most } \eta
\end{aligned}
$$

$\diamond$ Given $p(x)$ and $\mathcal{D}$, seek effective procedure ("compiler") to exhibit algorithm, or show one does not exist

## Examples in classical arithmetic over $\mathbb{R}^{n}$ (none work over $\mathbb{C}^{n}$ ).

- $M_{2}(x, y, z)=z^{6}+x^{2} \cdot y^{2} \cdot\left(x^{2}+y^{2}-2 \cdot z^{2}\right)$
- Positive definite and homogeneous, easy to evaluate accurately
- $M_{3}(x, y, z)=z^{6}+x^{2} \cdot y^{2} \cdot\left(x^{2}+y^{2}-3 \cdot z^{2}\right)$
- Motzkin polynomial, nonnegative, zero at $|x|=|y|=|z|$

$$
\text { if } \begin{aligned}
& |x-z| \leq|x+z| \wedge|y-z| \leq|y+z| \\
p= & z^{4} \cdot\left[4\left((x-z)^{2}+(y-z)^{2}+(x-z)(y-z)\right)\right]+ \\
& +z^{3} \cdot\left[2 \left(2(x-z)^{3}+5(y-z)(x-z)^{2}+5(y-z)^{2}(x-z)+\right.\right. \\
& \left.\left.2(y-z)^{3}\right)\right]+ \\
& +z^{2} \cdot\left[(x-z)^{4}+8(y-z)(x-z)^{3}+9(y-z)^{2}(x-z)^{2}+\right. \\
& \left.8(y-z)^{3}(x-z)+(y-z)^{4}\right]+ \\
& +z \cdot\left[2 ( y - z ) ( x - z ) \left((x-z)^{3}+2(y-z)(x-z)^{2}+\right.\right. \\
& \left.\quad 2(y-z)^{2}(x-z)+(y-z)^{3}\right]+ \\
& +(y-z)^{2}(x-z)^{2}\left((x-z)^{2}+(y-z)^{2}\right) \\
\text { else } \quad & \ldots 2^{\# \text { vars }-1} \text { more analogous cases }
\end{aligned}
$$

- $M_{4}(x, y, z)=z^{6}+x^{2} \cdot y^{2} \cdot\left(x^{2}+y^{2}-4 \cdot z^{2}\right)$
- Impossible to evaluate accurately


## Sneak Peak.

## The variety,

$$
V(p)=\{x: p(x)=0\}
$$

plays a necessary role.

## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Allowable varieties in Classical Model of arithmetic.

Define basic allowable sets:

- $Z_{i}=\left\{x: x_{i}=0\right\}$,
- $S_{i j}=\left\{x: x_{i}+x_{j}=0\right\}$,
- $D_{i j}=\left\{x: x_{i}-x_{j}=0\right\}$.

A variety $V(p)$ is allowable if it can be written as a finite union of intersections of basic allowable sets.

Denote by

$$
\mathbf{G}(\mathbf{p})=\mathbf{V}(\mathbf{p})-\cup_{\text {allowable } \mathbf{A} \subset \mathbf{V}(\mathbf{p})} \mathbf{A}
$$

the set of points in general position.
$V(p)$ unallowable $\Rightarrow G(p) \neq \emptyset$.

## Necessary condition.

Theorem 1: $V(p)$ unallowable $\Rightarrow p$ cannot be evaluated accurately on $\mathbb{R}^{n}$ or on $\mathbb{C}^{n}$.
Theorem 2: On a domain $\mathcal{D}$, if $\operatorname{Int}(\mathcal{D}) \cap G(p) \neq \emptyset, p$ cannot be evaluated accurately.

Examples on $\mathbb{R}^{n}$, revisited.

- $p(x, y, z)=x+y+z$

UNALLOWABLE

- $M_{2}(x, y, z)=z^{6}+x^{2} \cdot y^{2} \cdot\left(x^{2}+y^{2}-2 \cdot z^{2}\right)$

ALLOWABLE, $V(p)=\{0\}$.

- $M_{3}(x, y, z)=z^{6}+x^{2} \cdot y^{2} \cdot\left(x^{2}+y^{2}-3 \cdot z^{2}\right)$

ALLOWABLE, $V(p)=\{|x|=|y|=|z|\}$

- $M_{4}(x, y, z)=z^{6}+x^{2} \cdot y^{2} \cdot\left(x^{2}+y^{2}-4 \cdot z^{2}\right)$


## UNALLOWABLE

- $V(\operatorname{det}($ Toeplitz $))$, UNALLOWABLE $\Rightarrow$ no accurate linear algebra for Toeplitz (need arbitrary precision arithmetic, as we will see later).


## Necessary condition, real and complex.

Theorem 1: $V(p)$ unallowable $\Rightarrow p$ cannot be evaluated accurately on $\mathbb{R}^{n}$ or on $\mathbb{C}^{n}$.
Theorem 2: On a domain $\mathcal{D}$, if $\operatorname{Int}(\mathcal{D}) \cap G(p) \neq \emptyset, p$ cannot be evaluated accurately.

## Sketch of proof.

Simplest case: non-branching, no data reuse (except for inputs), nondeterminism.

Algorithm can be represented as a tree with extra edges from the sources, each node corresponds to an operation $(+,-, \times)$, each node has a specific $\delta$, each node has two inputs, one output.

Let $x \in G(p)$ and define $\operatorname{Allow}(x)$ as the smallest allowable set containing $x$.

## Necessary condition, real and complex.

Theorem 1: $V(p)$ unallowable $\Rightarrow p$ cannot be evaluated accurately on $\mathbb{R}^{n}$ or on $\mathbb{C}^{n}$.
Theorem 2: On a domain $\mathcal{D}$, if $\operatorname{Int}(\mathcal{D}) \cap G(p) \neq \emptyset, p$ cannot be evaluated accurately.

## Sketch of proof, cont'd.

Key fact: for a positive measure set of $\delta$ s in $\delta$-space, a zero output can be "traced back" down the tree to "allowable" condition ( $x_{i}=0$ or $x_{i}+x_{j}=0$ ), or trivial one ( $x_{i}-x_{i}=0$ ).
So for a positive measure set of $\delta \mathrm{s}$, either

- $p_{\text {comp }}(x, \delta)$ is not 0 (though $p(x)=0$ ), or
- for all $y \in \operatorname{Allow}(x) \backslash V(p), p_{\text {comp }}(y, \delta)=0$ (though $\left.p(y) \neq 0\right)$.

In either case, the polynomial is not accurately evaluable arbitrarily close to $x$, q.e.d.

## Sufficient Condition, complex case.

Theorem. Let $p$ be a polynomial over $\mathbb{C}^{n}$ with integer coefficients. If $V(p)$ is allowable, then $p$ is accurately evaluable.

## Sketch of proof.

Can write

$$
p(x)=c \prod_{i} p_{i}(x)
$$

where $p_{i}(x)$ is a power of some $x_{j}$ or $x_{j} \pm x_{k}$, and $c$ is an integer; all operations are accurate.

## Sufficient Condition, complex case.

Theorem. Let $p$ be a polynomial over $\mathbb{C}^{n}$ with integer coefficients. If $V(p)$ is allowable, then $p$ is accurately evaluable.

## Sketch of proof.

Can write

$$
p(x)=c \prod_{i} p_{i}(x)
$$

where $p_{i}(x)$ is a power of some $x_{j}$ or $x_{j} \pm x_{k}$, and $c$ is an integer; all operations are accurate.

Corollary. If $p$ is a complex multivariate polynomial, $p$ is accurately evaluable iff $p$ has integer coefficients and $V(p)$ is allowable.

## Sufficient Condition, real case.

Trickier... Allowability not sufficient:

- $q=\left(u^{4}+v^{4}\right)+\left(u^{2}+v^{2}\right)\left(x^{2}+y^{2}+z^{2}\right), V(p)=\{u=v=0\}$ : allowable and accurately evaluable
- $p=\left(u^{4}+v^{4}\right)+\left(u^{2}+v^{2}\right)(x+y+z)^{2}, V(p)=\{u=v=0\}$ : allowable but NOT accurately evaluable!
- Has to do with locally dominant behavior (in this case, near the set $\{u=v=0\}$ ).


## Sufficient Condition, real case.

Trickier... Allowability not sufficient:

- $q=\left(u^{4}+v^{4}\right)+\left(u^{2}+v^{2}\right)\left(x^{2}+y^{2}+z^{2}\right), V(p)=\{u=v=0\}$ : allowable and accurately evaluable
- $p=\left(u^{4}+v^{4}\right)+\left(u^{2}+v^{2}\right)(x+y+z)^{2}, V(p)=\{u=v=0\}$ : allowable but NOT accurately evaluable!
- Has to do with locally dominant behavior (in this case, near the set $\{u=v=0\}$ ).

Theorem. If all "dominant terms" are accurately evaluable on $\mathbb{R}^{n}$ then $p$ is accurately evaluable. In non-branching case, if $p$ is accurately evaluable on $\mathbb{R}^{n}$, then so are all "dominant terms".

## What is dominance? Newton Polytope



$$
p(x, y, z)=y^{8} z^{12}+x^{2} y^{2} z^{16}+x^{8} z^{12}+x^{6} y^{14}+x^{10} y^{6} z^{4}
$$

Component of $V(p)$ where $\{x=y=0\}$

## What is dominance? Normal Fan

$$
\begin{aligned}
& p(x, y, z)=y^{8} z^{12}+x^{2} y^{2} z^{-0.0} 16^{\circ}+x^{8} z^{12}+x^{6} y^{14}+x^{10} y^{6} z^{4} \\
& \text { Component of } V(p) \text { where }\{x=y=0\}
\end{aligned}
$$

## What is dominance? First orthant of -(Normal Fan)



$$
p(x, y, z)=y^{8} z^{12}+x^{2} y^{2} z^{16}+x^{8} z^{12}+x^{6} y^{14}+x^{10} y^{6} z^{4}
$$

Component of $V(p)$ where $\{x=y=0\}$

## What is dominance? Labeling dominant terms



$$
p(x, y, z)=y^{8} z^{12}+x^{2} y^{2} z^{16}+x^{8} z^{12}+x^{6} y^{14}+x^{10} y^{6} z^{4}
$$

Component of $V(p)$ where $\{x=y=0\}$

What is dominance? $(x, y)$ regions where different terms dominant


$$
p(x, y, z)=y^{8} z^{12}+x^{2} y^{2} z^{16}+x^{8} z^{12}+x^{6} y^{14}+x^{10} y^{6} z^{4}
$$

Component of $V(p)$ where $\{x=y=0\}$

## Sufficient Condition, real case.

Trickier... Allowability not sufficient:

- $q=\left(u^{4}+v^{4}\right)+\left(u^{2}+v^{2}\right)\left(x^{2}+y^{2}+z^{2}\right), V(p)=\{u=v=0\}$ : allowable and accurately evaluable
- $p=\left(u^{4}+v^{4}\right)+\left(u^{2}+v^{2}\right)(x+y+z)^{2}, V(p)=\{u=v=0\}$ : allowable but NOT accurately evaluable!
- Has to do with locally dominant behavior (in this case, near the set $\{u=v=0\}$ ).

Theorem. If all "dominant terms" are accurately evaluable on $\mathbb{R}^{n}$ then $p$ is accurately evaluable. In non-branching case, if $p$ is accurately evaluable on $\mathbb{R}^{n}$, then so are all "dominant terms".

Need inductive procedure of testing accurate evaluability, but so far no clear induction parameter.

## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Allowable varieties in black-box arithmetic.

Define black-boxes: $q_{1}, q_{2}, \ldots, q_{k}$ are polynomials
$\mathcal{V}_{j}=\left\{V \neq \mathbb{R}^{n}: V\right.$ can be obtained from $q_{j}$ through Process A, below $\}$

## Process A:

Step 1. repeat and/or negate, or 0 out some of the inputs,
Step 2. of the remaining variables, keep some symbolic, and find the variety in terms of the others.

Example: $q_{1}(x, y)=x-y$ has (up to symmetry)

$$
\begin{gathered}
\mathcal{V}_{1}=\{\{x=0\},\{x-y=0\},\{x+y=0\}\}, \\
q_{2}(x, y, z)=x-y \cdot z \text { has (up to symmetry) } \\
\mathcal{V}_{2}=\{\{x=0\},\{y=0\} \cup\{z=0\},\{x=0\} \cup\{x=1\},\{x=0\} \cup\{x=-1\}, \\
\{x=0\} \cup\{y=1\},\{x=0\} \cup\{y=-1\},\left\{x-y^{2}=0\right\},\left\{x+y^{2}=0\right\}, \\
\{x-y z=0\},\{x+y z=0\}\} .
\end{gathered}
$$

Allowable varieties in black-box arithmetic.
Define black-boxes: $q_{1}, q_{2}, \ldots, q_{k}$ are polynomials $\mathcal{V}_{j}=\left\{V \neq \mathbb{R}^{n}: V\right.$ can be obtained from $q_{j}$ through Process A $\}$

Define basic allowable sets:

- $Z_{i}=\left\{x: x_{i}=0\right\}$,
- $S_{i j}=\left\{x: x_{i}+x_{j}=0\right\}$,
- $D_{i j}=\left\{x: x_{i}-x_{j}=0\right\}$,
- any $V$ for which there is a $j$ such that $V \in \mathcal{V}_{j}$.


## Allowable varieties in black-box arithmetic.

Define black-boxes: $q_{1}, q_{2}, \ldots, q_{k}$ are polynomials $\mathcal{V}_{j}=\left\{V \neq \mathbb{R}^{n}: V\right.$ can be obtained from $q_{j}$ through Process A $\}$

A variety $V(p)$ is allowable if it is a union of irreducible parts of finite intersections of basic allowable sets.

Denote by

$$
\mathbf{G}(\mathbf{p})=\mathbf{V}(\mathbf{p})-\cup_{\text {allowable } \mathbf{A} \subset \mathbf{V}(\mathbf{p})} \mathbf{A}
$$

the set of points in general position.
$V(p)$ unallowable $\Rightarrow G(p) \neq \emptyset$.

Necessary condition, real and complex.
Theorem 1: $V(p)$ unallowable $\Rightarrow p$ cannot be evaluated accurately on $\mathbb{R}^{n}$ or on $\mathbb{C}^{n}$.

Theorem 2: On a domain $\mathcal{D}$, if $\operatorname{Int}(\mathcal{D}) \cap G(p) \neq \emptyset, p$ cannot be evaluated accurately.

Sufficient condition, complex, for all $q_{j}$ irreducible. Theorem: If $V(p)$ is a union of intersections of sets $Z_{i}, S_{i j}, D_{i j}$, and $V\left(q_{j}\right)$, then $p$ is accurately evaluable.

Corollary: If all $q_{j}$ are affine, then $p$ is accurately evaluable iff $V(p)$ is allowable.

## Consequences for Numerical Linear Algebra.

- $V(\operatorname{det}($ Toeplitz $))$ contains irreducible factors of arbitrarily large degree $\Rightarrow$ no set of black-boxes of bounded degree will be sufficient for accurate evaluation $\Rightarrow$ need arbitrary precision arithmetic to do NLA accurately on Toeplitz matrices.
- Same argument shows that we cannot accurately evaluate many generalized Vandermonde matrices (Schur functions as determinants).
- Conjecture: if the class of structured matrices has displacement rank $\geq 2$, then accurate evaluation will not always be possible.


## Complexity of Accurate Algorithms for General Structured Matrices

| Type of matrix | $\operatorname{det} A$ | $A^{-1}$ | Any <br> minor | LDU | SVD | Sym <br> EVD |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: |
| Acyclic <br> (bidiagonal and other) | $n$ | $n^{2}$ | $n$ | $\leq n^{2}$ | $n^{3}$ | N/A |
| Total Sign Compound <br> (TSC) | $n$ | $n^{3}$ | $n$ | $n^{4}$ | $n^{4}$ | $n^{4}$ |
| Diagonally Scaled Totally <br> Unimodular (DSTU) | $n^{3}$ | $n^{5} ?$ | $n^{3}$ | $n^{3}$ | $n^{3}$ | $n^{3}$ |
| Weakly diagonally <br> dominant M-matrix | $n^{3}$ | $n^{3}$ | No | $n^{3}$ | $n^{3}$ | $n^{3}$ |
| Displace- <br> Cauchy <br> ment <br> Rank One | $n^{2}$ | $n^{2}$ | $n^{2}$ | $\leq n^{3}$ | $n^{3}$ | $n^{3}$ |
| Vandermonde | $n^{2}$ | No | No | No | $n^{3}$ | $n^{3}$ |
| Toeplitz | $n^{2}$ | No | No | No | $*$ | $*$ |

* $=$ "it depends"


## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Choosing a finite precision arithmetic model

- In finite precision, accuracy always possible, only question is cost
- Measure bit complexity in floating point: $(e, m) \equiv 2^{e} \cdot m$
- Contrasts between complexity in Floating Point and Fixed Point
- Repeated squaring can have exponential cost in Fixed, polynomial in Float
- Det(A) polynomial in Fixed [Clarkson], unknown in Float
- Witness for matrix singularity (null vector) in Float can have exponentially many bits
- Computing "middle bits" of $\prod_{i=1}^{n}\left(1+x_{i}\right)$ polynomial in Fixed, as hard as computing the permanent in Float
- Float seems more natural for attaining relative accuracy


## Cost implications for Accuracy in Floating Point

- If a problem is accurately evaluable in Classical Model, the same algorithm works in Float
- Each operation runs in in polynomial time in size of inputs
- Ex: Motzkin polynomial, eig(Vandermonde)
- If a problem is accurately evaluable in Black-Box Model, then if you build an accurate library to evaluate each
"black-box" operation, the same algorithm works in Float
- If each "black-box" operation is of bounded degree and \#terms, then each operation runs in polynomial time in size of inputs
- Ex: eig(discretized scalar elliption PDE), $x+y+z$
- If set of black-box operations of unbounded degree and \#terms, then cost may be exponential
- Ex: $\operatorname{det}($ Toeplitz)


## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Is it worth getting the right answer?

- If the answer is ill-conditioned, why bother?
- Many problems have enormous condition numbers, but moderate structured conditioned numbers
- Ex: Hilbert matrix: exponentially large condition number as $n$ grows
- But $H_{i j}=1 /\left(x_{i}+x_{j}\right)$ with $x_{i}=i-.5$ well-conditioned wrt $x()$.
- True for all structured matrix examples
- So high accuracy deserved!


## Getting the right answer: Outline

1. Problem statement and (more) motivating examples
2. Classical Model (CM) and Black-Box Model (BBM) of arithmetic
3. Necessary and sufficient conditions for accurate evaluation in CM
4. Necessary and sufficient conditions for accurate evaluation in BBM
5. Consequences for finite precision arithmetic
6. Is it worth getting the right answer? Conditioning
7. Open problems

## Open problems

- Complete the decision procedure (analyze the dominant terms) when the domain is $\mathbb{R}^{n}$ and $V(p)$ allowable.
- Narrow the necessity and sufficiency conditions for the black-box case
- Extend to semi-algebraic domains $\mathcal{D}$.
- Incorporate division, rational functions, perturbation theory.
- Conjecture (Demmel, '04): Accurate evaluation is possible iff condition number has only certain simple singularities (depend on reciprocal distance to set of ill-posed problems).
- Extend to interval arithmetic.
- Implement decision procedure to "compile" an accurate evaluation program given $p(x), \mathcal{D}$, and minimal set of "black boxes"


## Reference

For a survey with many other references, see:
"Accurate and efficient expression evaluation and linear algebra,"
J. Demmel, I. Dumitriu, O. Holtz, P. Koev,

Acta Numerica (2008), v. 17, pp 87-145

## Topics.

1. Getting the right answer

- At all? In polynomial time?
- Depends on the model of arithmetic

2. Getting the same answer

- When running same problem on two different machines?
- When running same problem twice on same machine?

3. Getting a fast answer

- Arithmetic is cheap, moving data is expensive
- How does this change algorithms?


## Why wouldn't you get the same answer?

- Run the same program twice on different machines
- Different floating point semantics, compilers, ...
- Run the same program twice on the same machine
- Floating point nonassociativity and dynamic scheduling of parallel tasks
- Who cares?
- Recent NA-Digest request for reproducible parallel sparse linear solver for use in a FEM package used by construction engineers with contractual obligations for reproducibility
- Subsequent informal survey of many users gave wide range of reasons for wanting reproducibility
- Debugging


## How do we attain reproducibility?

- Question is cost
- All machines becoming parallel, running sequentially not an option
- Just avoid dynamic scheduling?
- What if OS varies number of cores available?
- Always use the same reduction tree, independent of \# cores?
- Just get the correctly rounded answer?
- Opportunity for this community?
- See related talk on debugging by Guillaume Revy


## Topics.

1. Getting the right answer

- At all? In polynomial time?
- Depends on the model of arithmetic

2. Getting the same answer

- When running same problem on two different machines?
- When running same problem twice on same machine?

3. Getting a fast answer

- Arithmetic is cheap, moving data is expensive
- How does this change algorithms?


## Arithmetic is cheap, moving data is expensive.

- Time to do one floating point operation already hundreds of times faster than getting data from main memory, or from another processor
- Technology trends
- Arithmetic getting faster at $\approx 60 \% /$ year
- Communication bandwidth (moving data, either between levels of memory hierarchy or processors over a network) only improving at most 25\%/year;
- Latency worse


## Impact on Linear Algebra

- Impact on Direct Linear Algebra (LU, QR, eig, SVD, ...)
- Thm (Ballard, D., Holtz, Schwartz): Lower bound on communication for any of these problems
* Generalizes existing lower bounds for dense matmul
* Dense or sparse matrices, sequential or parallel
- LAPACK/ScaLAPACK communicate asymptotically more than lower bounds
- New algorithms do attain lower bounds - large speedups * Up to 8x measured, 80x predicted


## Impact on Linear Algebra

- Impact on Direct Linear Algebra (LU, QR, eig, SVD, ...)
- Thm (Ballard, D., Holtz, Schwartz): Lower bound on communication for any of these problems
* Generalizes existing lower bounds for dense matmul
* Dense or sparse matrices, sequential or parallel
- LAPACK/ScaLAPACK communicate asymptotically more than lower bounds
- New algorithms do attain lower bounds - large speedups * Up to 8x measured, 80x predicted
- Impact on Iterative Linear Algebra (Krylov Methods) - Ditto
- See bebop.cs.berkeley.edu for papers, www.cs.berkeley.edu/~demmel for short course


## Conclusion

Time to reengineer all linear algebra software!

## Conclusion

Time to reengineer all linear algebra software!

## Don't communic....

