Towards accurate polynomial evaluation

or

When can Numerical Linear Algebra be done accurately?

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Joint work with Ioana Dumitriu and Olga Holtz (UC Berkeley)

Outline

- 1. Motivation and goal(s).
- 2. Model of arithmetic and setting.
- 3. What is *allowable* in classical arithmetic.
- 4. Results for classical arithmetic, real and complex.
- 5. What is *allowable* in black-box arithmetic.
- 6. Results for black-box arithmetic, real and complex.
- 7. Other models of arithmetic.
- 8. Open problems / Future work.

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Goal

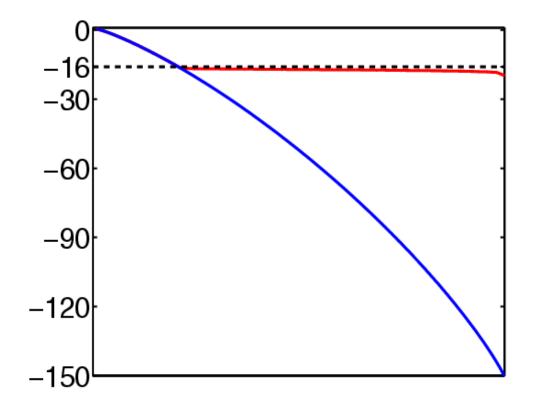
Given a family of structured matrices M(x), find **accurate** and **efficient** algorithms to solve linear algebra problems (eg $y = \det M(x)$ or $y = \operatorname{eig}(M(x))$), or prove that none exist

Accurately means relative error $\eta < 1$, i.e.

- $\diamond |y_{\text{computed}} y| \leq \eta |y|,$
- \diamond $\eta = 10^{-2}$ yields two digits of accuracy,
- \diamond $y_{\text{computed}} = 0 \iff y = 0.$

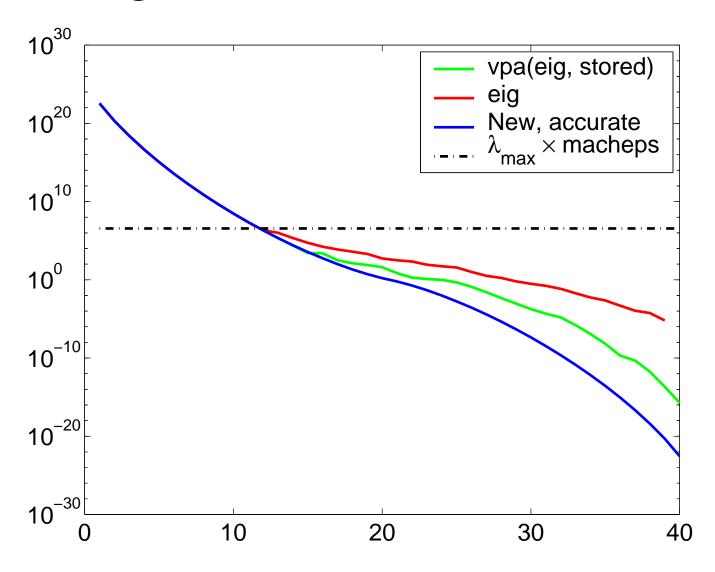
Efficiently means in polynomial time

Log₁₀(Eigenvalues) of 50x50 Hilbert Matrix

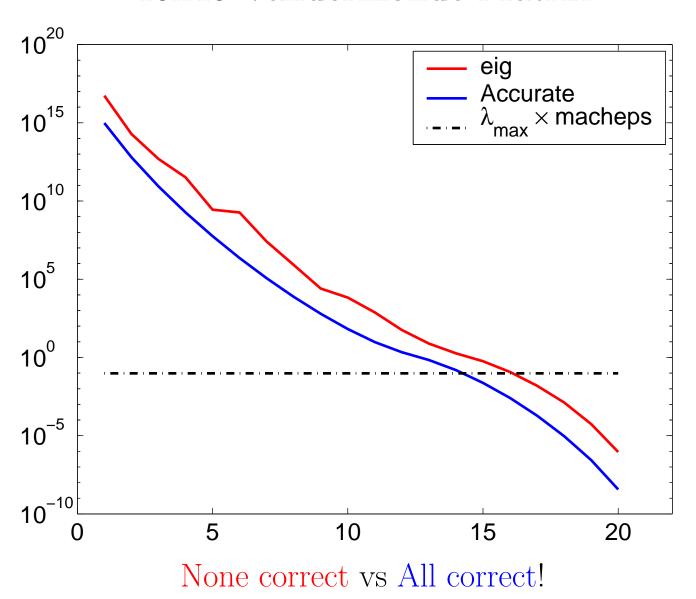


red line shows eigenvalues from conventional algorithm in 16 digits blue line shows eigenvalues from new algorithm in 16 digits Cost of guaranteed accuracy: $O(n^3 \log \kappa)$ vs $O(n^3 \log \log \kappa)$ where $\kappa = \text{condition number}$

Eigenvalues of 40x40 Pascal Matrix



Eigenvalues of 20x20 Schur complement of 40x40 Vandermonde Matrix



General Structured Matrices

				Any			Sym
Type of matrix		$\det A$	A^{-1}	minor	LDU	SVD	EVD
Acyclic							
(bidiagona)	l and other)						
Total Sign	Compound						
(TSC)							
Diagonally	Scaled Totally						
Unimodular (DSTU)							
Weakly diagonally							
dominant I	M-matrix						
	Cauchy						
Displace-							
ment Vandermonde							
Rank One							
	Polynomial						
	Vandermonde						
Toeplitz							

General Structured Matrices

				Any			Sym
Type of ma	$\det A$	A^{-1}	minor	LDU	SVD	EVD	
Acyclic		n	n^2	n	$\leq n^2$	n^3	N/A
(bidiagona	l and other)						
Total Sign	Compound	n	n^3	n	n^4	n^4	n^4
(TSC)							
Diagonally	n^3	n^{5} ?	n^3	n^3	n^3	n^3	
Unimodula							
Weakly dia	n^3	n^3	?	n^3	n^3	n^3	
dominant M-matrix							
	Cauchy	n^2	n^2	n^2	$\leq n^3$	n^3	n^3
Displace-							
ment	nent Vandermonde		?	?	?	n^3	n^3
Rank One							
	Polynomial	n^2	?	?	?	?	?
	Vandermonde						
Toeplitz		?	?	?	?	?	?

Totally Nonnegative Matrices

Type of			Any	y Gauss. elim.			NE	Ax=b		Eig.
Matrix	$\det A$	A^{-1}	minor	NP	PP	CP	NP		SVD	Val.
Cauchy										
Vandermonde										
Generalized										
Vandermonde										
Any TN in										
Neville form										

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Type of			Any	Gai	uss.	elim.	NE	Ax=b		Eig.
Matrix	$\det A$	A^{-1}	minor	NP			NP		SVD	Val.
Cauchy		n^2	n^2	n^2	n^3				n^3	
Vandermonde	n^2	n^3	n^3		n^2	1 -	n^2		n^3	n^3
Generalized	n^2	n^3	poly	n^2	n^2	poly	n^2	n^2	n^3	n^3
Vandermonde										
Any TN in	n	n^3	n^3	n^3	n^3	n^3	0	n^2	n^3	n^3
Neville form										

 $poly = poly(n, \lambda)$, where $\lambda = partition$

(see talk by Plamen Koev, Tuesday 4pm)

Reduce Matrix problem to Polynomial problem

Theorem: Being able to compute det(M) accurately is *necessary* to be able to compute LDU, eig, SVD, ... accurately

Theorem: Being able to compute all minors of M accurately is sufficient for computing M^{-1} , LDU, SVD, ... accurately

(Sufficient conditions for computing eig(M) accurately unknown in nonsymmetric, non-totally positive case)

Goal - restated

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.

- $\diamond |y_{\text{computed}} y| \leq \eta |y|,$
- \diamond $\eta = 10^{-2}$ yields two digits of accuracy,
- \diamond $y_{\text{computed}} = 0 \iff y = 0.$

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- o fl(a⊗b) = (a⊗b)(1+δ), with arbitrary roundoff error |δ| < ϵ ≪ 1- a, b and δ all real, or all complex
- Operations?

- \circ $fl(a\otimes b)=(a\otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon\ll 1$
- Operations?
 - \diamond in classical arithmetic, +, -, \times ; also exact negation;

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- Operations?
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 - How can we lose accuracy in this model?
 - * OK to multiply or add positive numbers
 - * OK to subtract exact numbers (initial data)
 - * Accuracy may only be lost when subtracting approximate results:

Recognizing Accuracy

- Ex: Compute $p(x) = x_1 + x_2 + x_3$
 - $-\mathbf{Try} \ alg(x,\delta) = ((x_1 + x_2)(1 + \delta_1) + x_3)(1 + \delta_2)$

$$rel_{-}err(x,\delta) = \frac{alg(x,\delta) - p(x)}{p(x)}$$

$$= \frac{x_1 + x_2}{x_1 + x_2 + x_3} (\delta_1 + \delta_2 + \delta_1 \cdot \delta_2) + \frac{x_3}{x_1 + x_2 + x_3} (\delta_2)$$

- $-\forall \epsilon > 0$, $rel_err(x, \delta)$ unbounded on an open subset of (x, δ) with $|\delta_i| < \epsilon$
- Generally: $rel_{-}err(x,\delta) = \sum_{r} \frac{p_{r}(x)}{p(x)} \cdot q_{r}(\delta)$
 - -Each $\frac{p_r(x)}{p(x)}$ must be bounded near p(x) = 0
- Ex: p(x) positive definite and homogeneous, degree d
 - If $p_r(x)$ also homogeneous, degree d, then $\frac{p_r(x)}{p(x)}$ bounded

- \circ $fl(a\otimes b)=(a\otimes b)(1+\delta)$, with arbitrary roundoff error $|\delta|<\epsilon\ll 1$
- Operations?
 - \diamond in classical arithmetic, +, -, \times ; also exact negation;
 - ♦ in black-box arithmetic, above plus selected polynomial expressions
 - * Ex: x yz (IBM's fused-multiply-add)
 - * Ex: wx yz (using double-double)
 - * Ex: small determinants (Shewchuk's Triangle)
 - * Ex: dot products (using Priest or Demmel/Hida algs)

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- Constants?

Availability of constants?

Example.

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

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

accurately.

- having no explicit constants no loss of generality for homogeneous, integer-coefficient polynomials.
- Black-box case:
 - any constants we choose can be accommodated via black-boxes

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 - non-determinism (because determinism is simulable)

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 - exact answer in finite # of steps in absence of roundoff error
 - branching based on comparisons
 - non-determinism (because determinism is simulable)
 - \diamond domains to be \mathbb{C}^n or \mathbb{R}^n (but some domain-specific results).

Problem Restatement

- ♦ Notation:
 - -p(x) multivariate polynomial to be evaluated, $x=(x_1,\ldots,x_k)$.
 - $-\delta = (\delta_1, \dots, \delta_m)$ is the vector of error (rounding) variables.
 - $-p_{comp}(x, \delta)$ is the result of algorithm to compute p at x with errors δ .
- \diamond Goal: Decide if \exists algorithm $p_{comp}(x, \delta)$ to accurately evaluate p(x) on \mathcal{D} :

```
\forall \ 0 < \eta < 1 ... for any \eta = desired relative error \exists \ 0 < \epsilon < 1 ... there is an \epsilon = maximum rounding error \forall \ x \in \mathcal{D} ... so that for all x in the domain \forall \ |\delta_i| \le \epsilon ... and for all rounding errors bounded by \epsilon |p_{comp}(x, \delta) - p(x)| \le \eta \cdot |p(x)| ... relative error is at most \eta
```

 \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).

•
$$M_2(x, y, z) = z^6 + x^2 \cdot y^2 \cdot (x^2 + y^2 - 2 \cdot z^2)$$

- Positive definite and homogeneous, easy to evaluate accurately

•
$$M_3(x, y, z) = z^6 + x^2 \cdot y^2 \cdot (x^2 + y^2 - 3 \cdot z^2)$$

- Motzkin polynomial, nonnegative, zero at |x| = |y| = |z|

if
$$|x-z| \leq |x+z| \wedge |y-z| \leq |y+z|$$

$$p = z^4 \cdot [4((x-z)^2 + (y-z)^2 + (x-z)(y-z))] +$$

$$+ z^3 \cdot [2(2(x-z)^3 + 5(y-z)(x-z)^2 + 5(y-z)^2(x-z) + 2(y-z)^3)] +$$

$$+ z^2 \cdot [(x-z)^4 + 8(y-z)(x-z)^3 + 9(y-z)^2(x-z)^2 + 8(y-z)^3(x-z) + (y-z)^4] +$$

$$+ z \cdot [2(y-z)(x-z)((x-z)^3 + 2(y-z)(x-z)^2 + 2(y-z)^2(x-z) + (y-z)^3] +$$

$$+ (y-z)^2(x-z)^2((x-z)^2 + (y-z)^2)$$
 else
$$... 2^{\# \text{vars}-1} \text{ more analogous cases}$$

•
$$M_4(x, y, z) = z^6 + x^2 \cdot y^2 \cdot (x^2 + y^2 - 4 \cdot z^2)$$

- Impossible to evaluate accurately

Sneak Peak.

The variety,

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

plays a necessary role.

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Define basic allowable sets:

- $\bullet Z_i = \{x : x_i = 0\},\$
- $\bullet S_{ij} = \{x : x_i + x_j = 0\},\$
- $\bullet D_{ij} = \{x : x_i x_j = 0\}.$

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

Denote by

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

the set of points in general position.

$$V(p)$$
 unallowable \Rightarrow $G(p) \neq \emptyset$.

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Necessary condition on V(p) for accurate evaluation of p

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 $Int(\mathcal{D}) \cap G(p) \neq \emptyset$, p cannot be evaluated accurately.

Examples on \mathbb{R}^n , revisited

- p(x, y, z) = x + y + z UNALLOWABLE
- $M_2(x, y, z) = z^6 + x^2 \cdot y^2 \cdot (x^2 + y^2 2 \cdot z^2)$ ALLOWABLE, $V(p) = \{0\}.$
- $M_3(x, y, z) = z^6 + x^2 \cdot y^2 \cdot (x^2 + y^2 3 \cdot z^2)$ ALLOWABLE, $V(p) = \{|x| = |y| = |z|\}$
- $M_4(x, y, z) = z^6 + x^2 \cdot y^2 \cdot (x^2 + y^2 4 \cdot z^2)$ UNALLOWABLE
- $V(\det(\text{Toeplitz}))$, UNALLOWABLE \Rightarrow no accurate linear algebra for Toeplitz in classical arithmetic
- V(minor(Vandermonde)), UNALLOWABLE, but ok on positive orthant (TP matrices)

Necessary condition on V(p), 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 $Int(\mathcal{D}) \cap G(p) \neq \emptyset$, p cannot be evaluated accurately.

Sketch of proof.

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

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 δ , each node has two inputs, one output.

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

Necessary condition on V(p), real and complex.

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Sketch of proof, cont'd.

Key fact: for a positive measure set of δs in δ-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 δ s, either

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

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

Sufficient condition on V(p) for accurate evaluation of p, 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 on V(p) for accurate evaluation of p, complex case.

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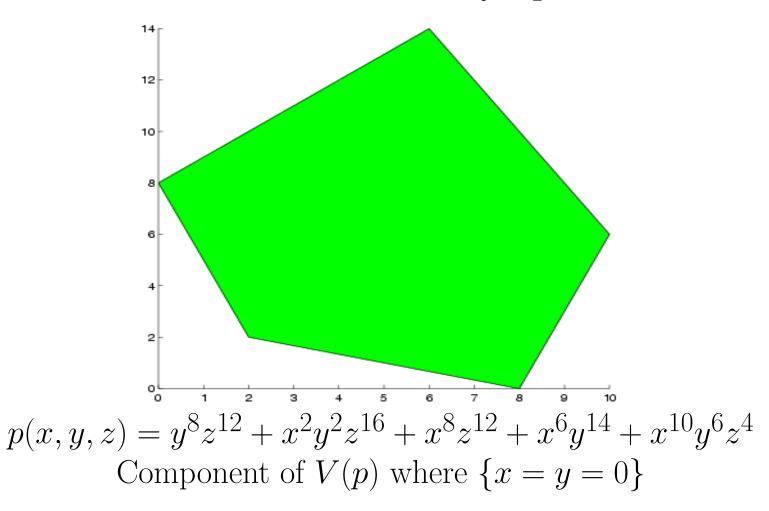
Corollary. If p is a complex multivariate polynomial, p is accurately evaluable iff p has integer coefficients and V(p) is allowable.

Sufficient condition for accurate evaluation, real case.

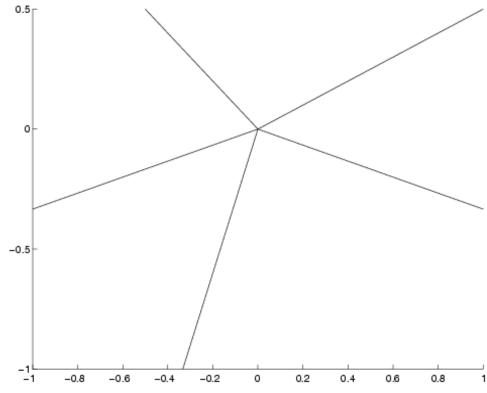
Trickier... Allowability (or any condition) of V(p) not sufficient:

- $q = (u^4 + v^4) + (u^2 + v^2)(x^2 + y^2 + z^2), V(p) = \{u = v = 0\}:$ allowable and accurately evaluable
- $p = (u^4 + v^4) + (u^2 + v^2)(x + y + z)^2$, $V(p) = \{u = v = 0\}$: allowable but NOT accurately evaluable!
- \bullet Say $p=(u^4+v^4)+(u^2+v^2)\hat{p}$ is "locally dominated" by \hat{p} near V(p)
 - Accurate evaluabilty of p depends on that of \hat{p}
 - Leads to induction on hierarchy of varieties and polynomials defined by "dominance"
 - Need to formally define dominance
 - Induction is work in progress

What is Dominance? Newton Polytope

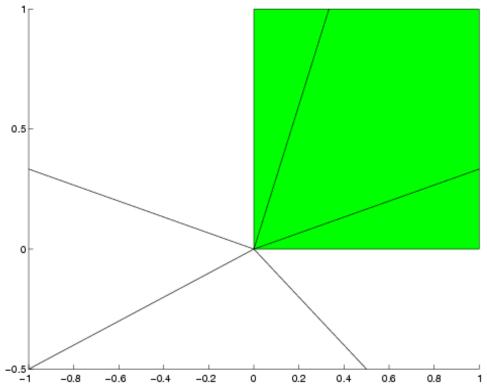


What is Dominance? Normal Fan



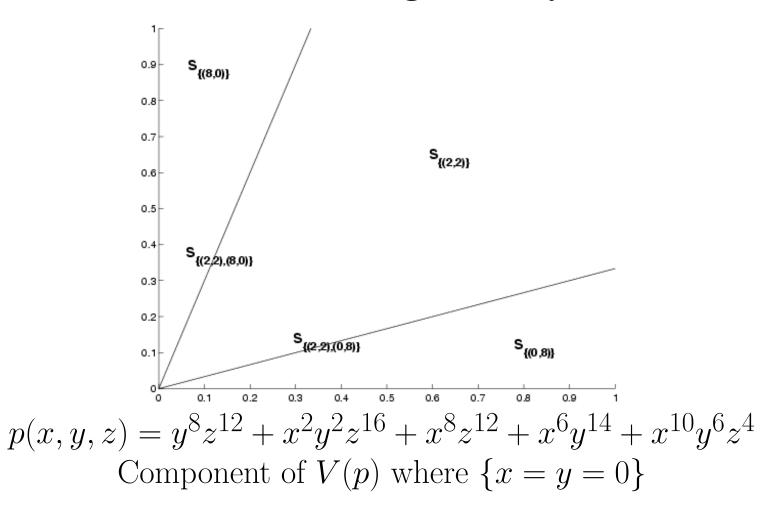
 $p(x,y,z) = y^8 z^{12} + x^2 y^2 z^{16} + x^8 z^{12} + x^6 y^{14} + x^{10} y^6 z^4$ Component of V(p) where $\{x=y=0\}$

What is Dominance? First orthant of -(Normal Fan)

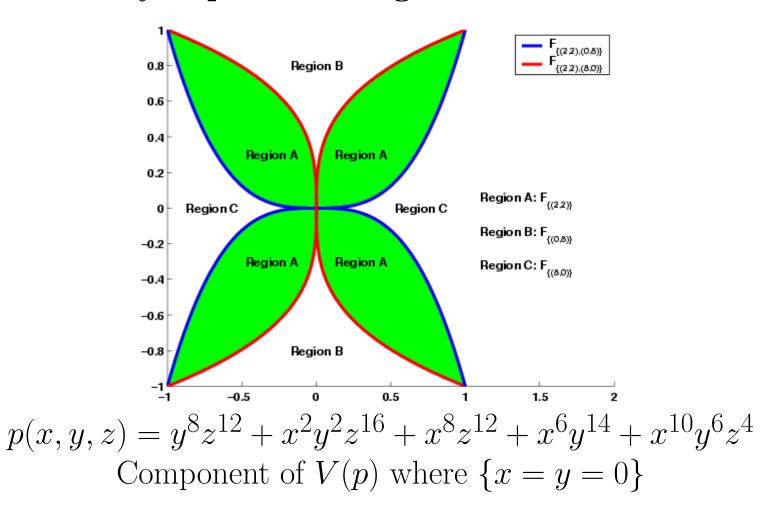


 $p(x,y,z) = y^8 z^{12} + x^2 y^2 z^{16} + x^8 z^{12} + x^6 y^{14} + x^{10} y^6 z^4$ Component of V(p) where $\{x=y=0\}$

What is Dominance? Labeling cones by dominant terms



What is Dominance? (x, y) regions where different terms dominate - by exponentiating cones



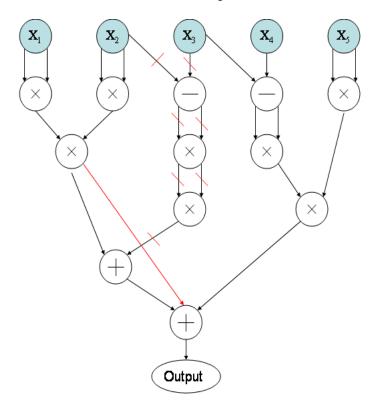
Sufficient condition for accurate evaluation, real case.

Trickier... Allowability not sufficient:

- $q = (u^4 + v^4) + (u^2 + v^2)(x^2 + y^2 + z^2), V(p) = \{u = v = 0\}:$ allowable and accurately evaluable
- $p = (u^4 + v^4) + (u^2 + v^2)(x + y + z)^2$, $V(p) = \{u = v = 0\}$: allowable but NOT accurately evaluable!
- Say $p = (u^4 + v^4) + (u^2 + v^2)\hat{p}$ is "locally dominated" by \hat{p} near V(p)

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".

Sketch of showing that accurate evaluation of dominant terms is necessary for accurate evaluation of p



Pruning is used to create accurate algorithm for any dominant term from accurate algorithm for p

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Allowable varieties in black-box arithmetic

Define **black-boxes** q_1, q_2, \ldots, q_k polynomial operations with various inputs, and for any j,

 $\mathcal{V}_j = \{V \neq \mathbb{R}^n : V \text{ can be obtained from } q_j \text{ through } \mathbf{Process } \mathbf{A}, \text{ below} \}$

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) $\mathcal{V}_1 = \{\{x = 0\}, \{x - y = 0\}, \{x + y = 0\}\},$ $q_2(x, y, z) = x - y \cdot z \text{ has (up to symmetry)}$

$$\mathcal{V}_2 = \{ \{x = 0\}, \{y = 0\} \cup \{z = 0\}, \{x = 0\} \cup \{x = 1\}, \{x = 0\} \cup \{x = -1\}, \{x = 0\} \cup \{y = 1\}, \{x = 0\} \cup \{y = -1\}, \{x - y^2 = 0\}, \{x + y^2 = 0\}, \{x - yz = 0\}, \{x + yz = 0\} \}.$$

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Define basic allowable sets:

- $\bullet Z_i = \{x : x_i = 0\},\$
- $\bullet S_{ij} = \{x : x_i + x_j = 0\},\$
- $\bullet D_{ij} = \{x : x_i x_j = 0\},\$
- any V for which there is a j such that $V \in \mathcal{V}_j$.

Allowable varieties in black-box arithmetic

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$$\mathcal{V}_j = \{V \neq \mathbb{R}^n : V \text{ can be obtained from } q_j \text{ through } \mathbf{Process } \mathbf{A} \}$$

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

Denote by

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

the set of points in general position.

$$V(p)$$
 unallowable \Rightarrow $G(p) \neq \emptyset$.

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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 $Int(\mathcal{D}) \cap G(p) \neq \emptyset$, p cannot be evaluated accurately.

Sufficiency condition, complex, for all q_j irreducible.

Theorem: If V(p) is a union of intersections of sets Z_i , S_{ij} , D_{ij} , and $V(q_i)$, then p is accurately evaluable.

Corollary: If all q_j are affine, then p is accurately evaluable iff V(p) is allowable.

General Structured Matrices

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

* = it depends on polynomial (eg orthogonal ok)

Other linear algebra consequences

- Let $M_n(x)$ be a family of n-by-n structured matrices
- Thm: If $\det(M_n(x))$ has an irreducible factor $p_n(x)$ over \mathbb{C} whose degree grows with n, then no set of "black-boxes" of bounded degree can accurately evaluate all $\det(M_n(x))$ over \mathbb{C} .
- Cor: $\det(\text{Toeplitz}_n(x))$ cannot be evaluated accurately by any set of "black-boxes" of bounded degree over \mathbb{C} .
- Thm: If $V_{\mathbb{R}}(\det(M_n(x)))$ has a regular point at which the tangent depends on a growing number of coordinates, then no set of "blackboxes" of bounded degree can accurately evaluate all $\det(M_n(x))$ over \mathbb{R} .
- Cor: $\det(\text{Toeplitz}_n(x))$ cannot be evaluated accurately by any set of "black-boxes" of bounded degree over \mathbb{R} .
- Accurate Toeplitz matrix computations need "infinite precision"
- What other $M_n(x)$ share these properties?

Outline

- 1. Motivation and goal(s).
- 2. Model of arithmetic and setting.
- 3. What is *allowable* in classical arithmetic.
- 4. Results for classical arithmetic, real and complex.
- 5. What is *allowable* in black-box arithmetic.
- 6. Results for black-box arithmetic, real and complex.
- 7. Other models of arithmetic
- 8. Open problems / Future work.

Other Models of arithmetic

- Other models of real arithmetic
 - Blum/Shub/Smale, Cucker/Smale, Pour-El/Richards
- Comparing Reals and Integers
 - Reals, with rounded arithmetic as described
 - * Some (most) p(x) impossible to evaluate accurately
 - Integers, with bit operations (usual Turing machine)
 - * All p(x) evaluable exactly, only question is cost
 - $* \det(M)$ evaluable in polynomial time
 - * Not a good bit model for real arithmetic

A bit model for Reals

- $x = m \cdot 2^e$, m and e integers, with bit operations
- Still a Turing machine, but inputs better capture reals
- Models floating point arithmetic
- All p(x) evaluable exactly, but cost can be much higher
- Cost of arbitrary bit of $\prod_i (1+2^{e_i})$ same as permanent
- Cost of x + y + z exponential unless done carefully (next slide)
- \bullet Cost of det(M) unknown, even for tridiagonal
- Cost of new matrix algorithms exponentially lower than conventional algorithms to guarantee same accuracy
 - $-\log\log\kappa$ vs $\log\kappa$
 - $-\log \log \kappa$ is polynomial in size of input

Adding Numbers in Bit Model of Arithmetic

- $x = m \cdot 2^e$ where m and e are integers
- Cancellation is obstable to accuracy:
 - $-(2^e+1)-2^e$ requires e bits of intermediate precision
 - Not polynomial time in size of input $\log_2 e$
- "Sort and Sum" Algorithm for $S = \sum_{i=1}^{n} x_i$

Sort so
$$|e_1| \ge |e_2| \ge \cdots \ge |e_n|$$
 ... $|x_1| \ge \cdots \ge |x_n|$ more than enough $S = 0$... $B > b$ bits for $i = 1$ to n $S = S + x_i$

- Thm: Let $N = 1 + 2^{B-b} + 2^{B-2b} + \cdots + 2^{B \mod b} = 1 + \lceil \frac{2^{B-b}}{1-2^{-b}} \rceil$. Then
 - If $n \leq N$, then S accurate to nearly b bits, despite any cancellation
 - If $n \ge N + 2$, then S may be completely wrong (wrong sign)
 - If n = N + 1, in between these cases, depending on underflow
- Ex: x_i double (b = 53), S extended $(B = 64) \Rightarrow N = 2049$

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Open problems / Future work.

- 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} .
- Apply to more structured matrix classes
- **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"