Validated numerics for algebraic path tracking

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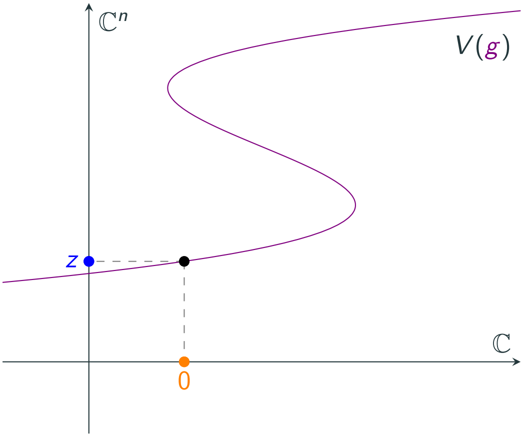
Introduction

Setup

- Let $g : \mathbb{C} \times \mathbb{C}^n \to \mathbb{C}^n$ be a polynomial map.
- Notation: $g_t : \mathbb{C}^n \to \mathbb{C}^n$ defined by $g_t(z) = g(t, z)$.
- Let $z \in \mathbb{C}^n$ such that $g_0(z) = 0$.



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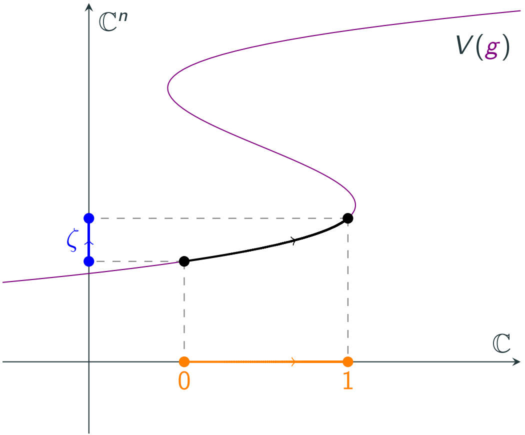
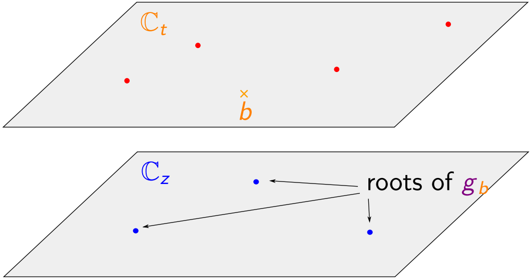
- Let $z \in \mathbb{C}^n$ such that $g_0(z) = 0$.

$\rightsquigarrow$ Moving the parameter from 0 to 1 induces $\zeta : [0, 1] \to \mathbb{C}^n$ s.t. $\zeta(0) = z$ and $g_t(\zeta(t)) = 0$.

- Goal: "Track" ζ, with some topological guarantees.



Motivation: braid computations



Setup

- Let $g \in \mathbb{C}[t, z]$,
- let $b \in \mathbb{C} \setminus \Sigma$ be a base point,

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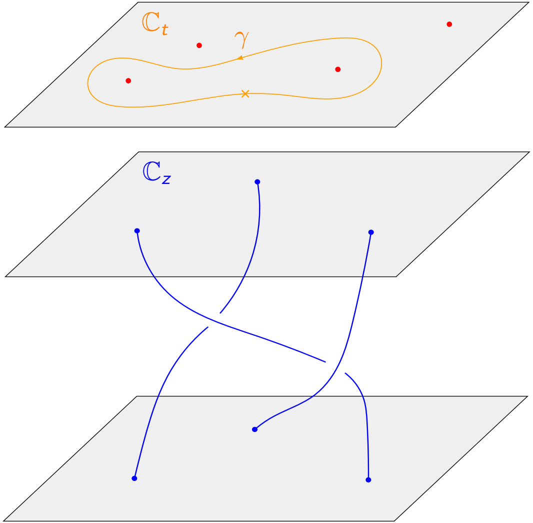


Setup

- Let $g \in \mathbb{C}[t, z]$,
- let $b \in \mathbb{C} \backslash \Sigma$ be a base point,
- let $\gamma : [0, 1] \to \mathbb{C} \backslash \Sigma$ be a loop starting at b.
- The displacement of all roots of g_t when t moves along γ defines a braid.

Algorithmic goal

Input: g, γ (p.w. linear)

Output: the associated braid

Tool: certified path tracking

Previous work

Noncertified path trackers

- PHCpack by Verschelde (1999)
- Bertini by Bates, Hauenstein, Sommese, and Wampler (2013)
- HomotopyContinuation.jl by Breiding and Timme (2018)

Certified path trackers using Smale's alpha-theory

- NAG for M2 by Beltrán and Leykin (2012, 2013)

Certified path trackers in one variable

- Marco-Buzunariz and Rodríguez (2016)
- Kranich (2015)
- Xu, Burr, and Yap (2018)

Certified path trackers using interval arithmetic

- Kearfott and Xing (1994)
- van der Hoeven (2015) *Krawczyk operator + Taylor models*
- Duff and Lee (2024) *similar to us but independent work*

Contributions

- Specify an *algorithm* implementing the Krawczyk + Taylor approach.
- Prove *termination*.
- In which model?
  - Exact arithmetic is not realistic.
  - We can't prove anything with 64-bits floating point numbers.
  - We want an adaptive precision model (as implemented by MPFI or Arb).

  $\rightsquigarrow$ We have to recognize when the working precision may not be enough.

- How good is the Krawczyk + Taylor approach?

  $\rightsquigarrow$ Competitive Rust implementation

Interval arithmetic

Problem

Given $f \in \mathbb{R}[x]$, I and J intervals, check $f(\mathrm{I}) \subseteq \mathrm{J}$.

Sufficient solution

- Define interval binary operations $\boxplus$ and $\boxtimes$ that take two intervals, give an interval and is such that for all $x \in \mathrm{I}$, $y \in \mathrm{J}$,

$$x + y \in \mathrm{I} \boxplus \mathrm{J}, \; xy \in \mathrm{I} \boxtimes \mathrm{J}$$

- Write f as a composition of binary operations and replace each operation by its interval counterpart (**interval extension**, denoted by $\square f$), then plug I and check if the result is contained in J.

! This is only a sufficient condition

Computational model

- Interval endpoints : $\mathbb{Q}$,
- $[a, b] \boxplus [c, d] = [a + c, b + d]$,
- $[a, b] \boxtimes [c, d] = [\min\{ac, ad, bc, bd\}, \max\{ac, ad, bc, bd\}]$.

Pros and cons

✔ good theoritical properties

✘ coefficient swell

Computational model

- Interval endpoints : {IEEE-754 64-bits floating-point numbers},
- $[a, b] \boxplus [c, d] = [\underline{a + c}, \overline{b + d}]$,
- $[a, b] \boxtimes [c, d] = [\min\{\underline{ac}, \underline{ad}, \underline{bc}, \underline{bd}\}, \max\{\overline{ac}, \overline{ad}, \overline{bc}, \overline{bd}\}]$.

Pros and cons

✔ fast

✘ bad theoritical properties

✘ not enough representable numbers

Computational model

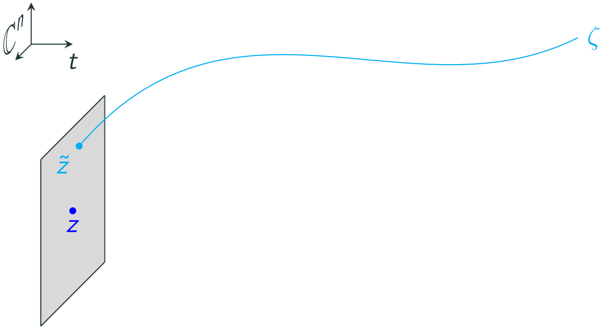
- Interval endpoints : $\{m2^e \in \mathbb{R} : m, e \in \mathbb{Z}\}$,
- $[a, b] \boxplus_u [c, d] \subseteq [a + c - Mu, b + d + Mu]$,
- $[a, b] \boxtimes_u [c, d] \subseteq [\min\{ac, ad, bc, bd\} - M^2 u, \max\{ac, ad, bc, bd\} + M^2 u]$,

for all $M \geq 1$, all $a, b, c, d \in [-M, M]$, and $u \in (0, 1)$ is the unit roundoff that should be specified at each operation.

Pros and cons

- ✔ good theoritical properties as $u \to 0$
- ✔ fast when we can maintain low precision
- implemented by MPFI and Arb
- compatible with IEEE-754 floating point arithmetic, when $u > 2^{-53}$
- when implemented with double precision only, a computation is guaranteed to terminate or fail with a precision error, it cannot hang

The folklore meta-algorithm



“Algorithm”

```
def track(g, Z):
    t ← 0
    L ← []
    while t < 1:
        Z ← refine(g_t, Z)
        pred ← a predictor
        δ ← validate(g, t, Z, pred)
        t ← t + δ
        append (t, Z) to L
    return L
```

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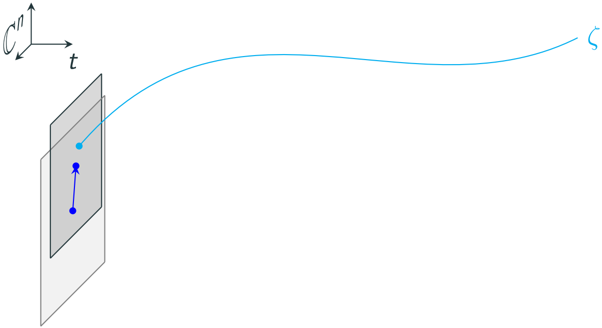

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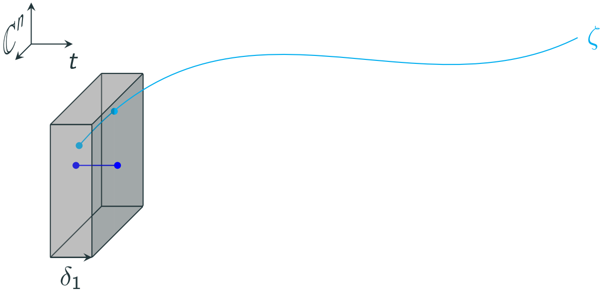

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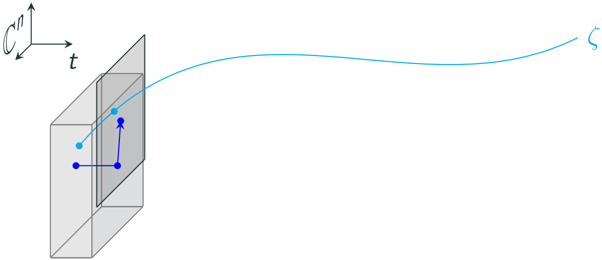

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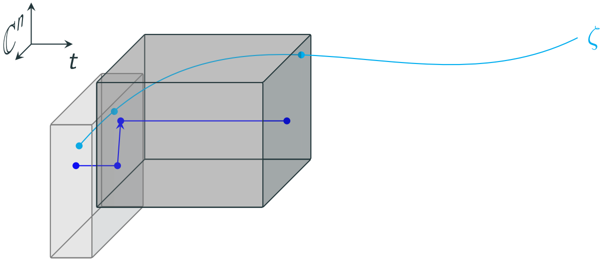

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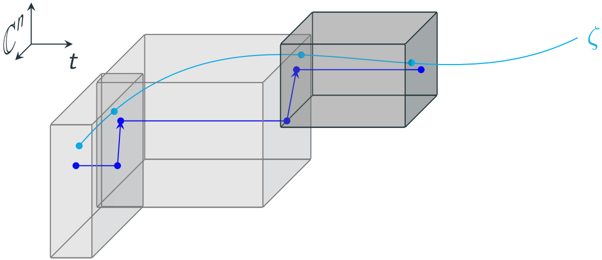

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Moore boxes, the datastructure for isolating boxes

Root isolation criterion (Krawczyk (1969), Moore (1977), Rump (1983))

- $f : \mathbb{C}^n \to \mathbb{C}^n$ polynomial, $\rho \in (0, 1)$,
- $z \in \mathbb{C}^n$, $A \in \mathbb{C}^{n \times n}$, $B \subseteq \mathbb{C}^n$ a ball of center 0,

such that for all $u, v \in B$,

$$-Af(z) + [\mathrm{I}_n - A \cdot Jf(z + u)]v \in \rho B.$$

Then f has a unique zero in $z + \rho B$.

Moore boxes, the datastructure for isolating boxes

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Then f has a unique zero in $z + \rho B$.

Proof sketch

We show that $\varphi : z + \rho B \to \mathbb{C}^n$ defined by $\varphi(w) = w - Af(w)$ is a ρ-contraction map with values in $z + \rho B$.

Definition

A ρ-Moore box for f is a triple (z, B, A) which satisfies Moore's criterion.

Refinement of Moore boxes

Algorithm

def *refine*(f, z, B, A):
    $U \leftarrow A$; $B \leftarrow 2B$
    while not $-A \cdot \Box f(z) + [I - A \cdot \Box Jf(z + B)]\, B \subseteq \frac{1}{8} B$
        if $-U \cdot \Box f(z) \subseteq \frac{1}{512} B$: # left term is small
            $B \leftarrow \frac{1}{2} B$
        else: # left term is big
            $z \leftarrow z - U f(z)$
        $A \leftarrow Jf(z)^{-1}$ # unchecked arithmetic
    return z, B, A

Input

- $f : \mathbb{C}^n \to \mathbb{C}^n$ polynomial,
- z, B, A a $\frac{7}{8}$-Moore box for f.

Output

A $\frac{1}{8}$-Moore box for f with same associated zero as z, B, A.

Refinement of Moore boxes

Algorithm

def *refine*(f, z, B, A):
  $U \leftarrow A$; $B \leftarrow 2B$; shrink_cnt $\leftarrow 0$
  while not $-A \cdot \square f(z) + [I - A \cdot \square Jf(z+B)]\, B \subseteq \frac{1}{8} B$
    if $-U \cdot \square f(z) \subseteq \frac{1}{512} B$: # left term is small
      $B \leftarrow \frac{1}{2} B$; shrink_cnt $\leftarrow$ shrink_cnt $+ 1$
      if shrink_cnt > 8:
        double working precision
    else: # left term is big
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      if shrink_cnt > 8:
        double working precision
    else: # left term is big
      $\delta \leftarrow U \cdot \square f(z)$
      if *width*$(z - \delta) > \frac{1}{40} \|\delta\|_{\square}$:
        double working precision
      else:
        $z \leftarrow$ *mid*$(z - \delta)$
    $A \leftarrow Jf(z)^{-1}$ # unchecked arithmetic
  return z, B, A

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A $\frac{1}{8}$-Moore box for f with same associated zero as z, B, A.

Proposition

refine terminates and is correct.

Step validation

Input

- $g : \mathbb{C} \times \mathbb{C}^n \to \mathbb{C}^n$,
- $t \in [0, 1]$,
- (z, B, A) a $\frac{1}{8}$-Moore box for g_t, returned by refine.

Output

$\delta > 0$ s.t. for all $s \in T = [t, t + \delta]$, (z, B, A) is a $\frac{7}{8}$-Moore box for g_s.

Proposition

validate terminates and is correct.

Algorithm

def *validate*$(g, t, \delta_{\mathrm{hint}}, z, B, A)$**:**

 $\delta \leftarrow \delta_{\mathrm{hint}}$; $\quad T \leftarrow [t, t + \delta]$

 while $-A \cdot \Box g_T(z) + [I - A \cdot \Box J g_T(z + B)]\, B \not\subseteq \frac{7}{8} B$**:**

  $\delta \leftarrow \frac{\delta}{2}$; $\quad T \leftarrow [t, t + \delta]$

  if $\delta < u$**:**

   double working precision

 return δ

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    if $\delta < u$**:**

      double working precision

  return δ

Remark

It is possible to modify this algorithm to validate along a predictor. It requires the use of Taylor models.

Implementation

- ✓ Rust implementation.
- ✓ Available at https://gitlab.inria.fr/numag/algpath.
- ✗ Double precision only, abort instead of raising precision.
- ✓ SIMD interval arithmetic, following Lambov (2008).
- ✓ Hermite's cubic predictor.
- ✓ Benchmarked against HomotopyContinuation.jl and NAG for Macaulay2.

We have benchmarks, but caveat

- They may not be relevant for your application.
- Timings are difficult to get consistent, especially with Julia.
- Large variability of the metrics.

So, is it fast?

Total time

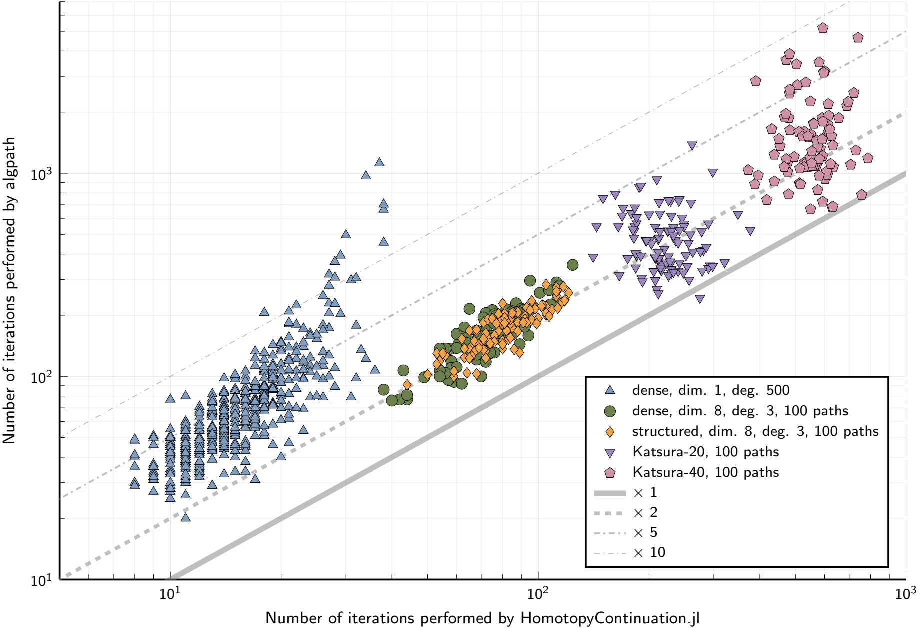
- 1-30× slower than HC.jl, lot of variability
- orders of magnitude faster than M2

Iterations/sec. (measure the efficiency *refine* and *validate*)

- ❗ 2× slower than M2 (I have been surprised by the efficiency of M2!)
- 5-10× slower than HC.jl

Total number of iterations (measure the theoretical merit)

- ❗ 1-5× more iterations than HC.jl + large deviations
- orders of magnitude less than M2
- ❗ 1-8× the theoretical minimum of the method (this has a precise meaning)
- Maybe we can gain a factor 2 by imitating Duff and Lee (2024).



Number of iterations performed by algpath
Number of iterations performed by HomotopyContinuation.jl
10^1
10^2
10^3
dense, dim. 1, deg. 500
dense, dim. 8, deg. 3, 100 paths
structured, dim. 8, deg. 3, 100 paths
Katsura-20, 100 paths
Katsura-40, 100 paths
× 1
× 2
× 5
× 10

				circuit size		HomotopyContinuation.jl					algpath					Macaulay2				
name	dim.	deg	# paths	f	$\mathrm{d}f$	fail.	med.	max.	ksteps/s	time	fail.	med.	max.	ksteps/s	time	fail.	med.	max.	ksteps/s	time
dense	1	30	30	248	314		10	25	41	2.0		23	372	25	< 0.1		830 k	3478 k	30	18 min
dense	1	40	40	328	416		14	30	45	2.0		34	197	24	< 0.1			> 1 h		
dense	1	50	50	408	520		12	61	37	1.9		30	5567	13	0.7			> 1 h		
dense	1	100	100	808	1054		13	51	23	1.9		38	5289	7.4	1.4			> 1 h		
dense	1	500	500	4008	5466		14	59	3.8	3.9	2	60	1121	2.3	17	500				4.0
dense	1	1000	1000	8008	10952		15	100	1.7	12	35	74	976	1.1	82	1000				29
dense	2	10	100	1016	1280		22	74	33	2.6		53	307	9.2	0.7		33 k	301 k	28	158
dense	2	20	400	3616	4612		25	63	13	3.1		74	401	2.9	12			> 1 h		
dense	2	30	900	7816	9952		24	127	5.8	6.4		85	690	1.4	72			> 1 h		
dense	2	40	1600	13616	17284		25	95	3.4	14		100	998	0.81	268			> 1 h		
dense	2	50	2500	21016	26624		27	84	2.3	33		117	1675	0.53	12 min			> 1 h		
katsura	9	2	256	448	228		82	132	54	4.2		148	286	9.5	4.2		12 k	59 k	18	186
katsura	11	2	1024	606	308		100	179	41	6.7		177	359	6.3	30		21 k	88 k	13	30 min
katsura	16	2	32768	1090	548		153	303	22	235		304	1847	2.7	1 h			> 50 h		
katsura	21	2	1048576	1696	844		209	469	13	4 h	483	427	8798	1.4	101 h			not benchmarked		
katsura *	26	2	100	2430	1202		305	466	6.9	8.8	1	800	2930	0.73	125			> 1 h		
katsura *	31	2	100	3286	1614		382	538	4.9	12	1	852	5021	0.47	219			> 1 h		
katsura *	41	2	100	5376	2618		554	787	2.7	24	9	1371	5182	0.19	13 min			> 1 h		
dense *	4	3	100	1080	1318		39	67	41	2.4		66	127	8.3	0.9		3384	9936	35	10
dense *	6	3	100	4092	5384		54	96	9.0	3.3		112	224	2.3	5.1		11 k	24 k	18	62
dense *	8	3	100	11120	15242		73	124	2.1	6.3		157	354	0.86	19		21 k	74 k	9.5	243
structured *	4	3	100	244	418		40	78	92	4.0		75	199	24	0.4		4531	8925	41	11
structured *	6	3	100	426	778		66	101	59	3.9		130	254	13	1.1		18 k	61 k	23	85
structured *	8	3	100	670	1252		81	121	40	3.9		182	283	7.9	2.3		36 k	97 k	13	305
structured ^{N}	5	5	1	302	545		42	42	4.9	3.1		99	99	18	< 0.1		252 k	252 k	12	22
structured ^{N}	10	10	1	1034	2024		53	53	0.18	3.1		123	123	4.9	< 0.1			> 1 h		
structured ^{N}	15	15	1	2366	5079			> 8 GB				628	628	2.0	0.4			> 8 GB		
structured ^{N}	20	20	1	3554	6721			> 8 GB				1591	1591	1.2	1.5			> 8 GB		
structured ^{N}	25	25	1	5466	10541			> 8 GB				1734	1734	0.69	2.9			> 8 GB		
structured ^{N}	30	30	1	7788	15239			> 8 GB				1989	1989	0.43	5.2			> 8 GB		

			HomotopyContinuation.jl			algpath			Macaulay2		
name	dim.	max deg	med.	ksteps/s	time (s)	med.	ksteps/s	time (s)	med.	ksteps/s	time (s)
dense	1	10	6	30	1.8	11	55	< 0.1	629	55	0.2
dense	1	50	12	37	1.9	30	13	0.7		> 1 h	
dense	2	10	22	33	2.6	53	9.2	0.7	33 k	28	158
dense	2	30	24	5.8	6.4	85	1.4	72		> 1 h	
dense	2	50	27	2.3	33	117	0.53	12 min		> 1 h	
katsura	9	2	82	54	4.2	148	9.5	4.2	12 k	18	186
katsura	11	2	100	41	6.7	177	6.3	30	21 k	13	30 min
katsura	16	2	153	22	235	304	2.7	1 h		> 50 h	
katsura	21	2	209	13	4 h	427	1.4	101 h		not benchmarked	
dense *	8	3	73	2.1	6.3	157	0.86	19	21 k	9.5	243
structured *	8	3	81	40	3.9	182	7.9	2.3	36 k	13	305
structured $^{\mathrm{N}}$	10	10	53	0.18	3.1	123	4.9	< 0.1		> 1 h	
structured $^{\mathrm{N}}$	20	20		> 8 GB		1591	1.2	1.5		> 8 GB	
structured $^{\mathrm{N}}$	30	30		> 8 GB		1989	0.43	5.2		> 8 GB	

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Test data

We tested systems of the form $g_t(z) = tf^{\odot}(z) + (1-t)f^{\triangleright}(z)$ ($f^{\triangleright}$ is the start system, $f^{\odot}$ is the target system).

Test data

We tested systems of the form $g_t(z) = t f^{\odot}(z) + (1-t) f^{\triangleright}(z)$ ($f^{\triangleright}$ is the start system, $f^{\odot}$ is the target system).

Target systems

- Dense: $f_i^{\odot}$'s of given degree with random coefficients
- Structured: $f_i^{\odot}$'s of the form $\pm 1 + \sum_{i=1}^{5} \left(\sum_{j=1}^{n} a_{i,j} z_j \right)^d$, $a_{i,j} \in_R \{-1, 0, 1\}$
- Katsura family (sparse - high dimension - low degree)

Test data

We tested systems of the form $g_t(z) = tf^{\odot}(z) + (1-t)f^{\triangleright}(z)$ ($f^{\triangleright}$ is the start system, $f^{\odot}$ is the target system).

Target systems

- Dense: $f_i^{\odot}$'s of given degree with random coefficients
- Structured: $f_i^{\odot}$'s of the form $\pm 1 + \sum_{i=1}^{5} \left(\sum_{j=1}^{n} a_{i,j} z_j \right)^d$, $a_{i,j} \in_R \{-1, 0, 1\}$
- Katsura family (sparse - high dimension - low degree)

Start systems

- Total degree homotopies: $f_i^{\triangleright}$'s of the form $\gamma_i(z_i^{d_i} - 1)$, $\gamma_i \in_R \mathbb{C}$, $d_i = \deg f_i^{\odot}$
- Newton homotopies: $f^{\triangleright}(z) = f^{\odot}(z) - f^{\odot}(z_0)$