Numerical algebraic geometry

Jonathan Hauenstein

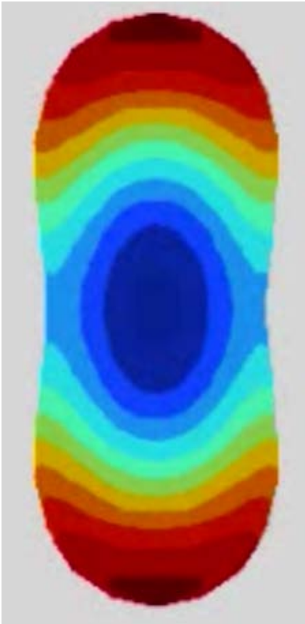
Convex Algebraic Geometry
BIRS
February 16, 2010

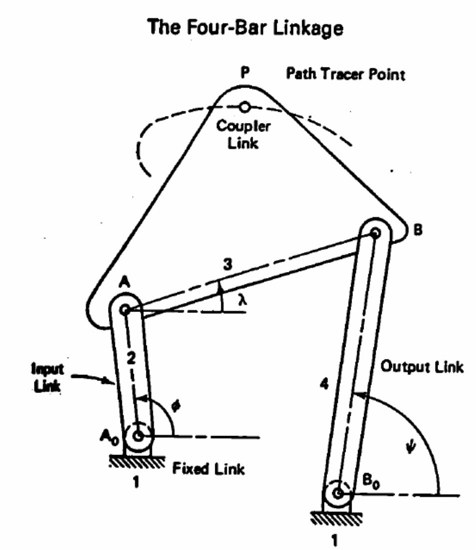
Example applications

Inverse 6R problem

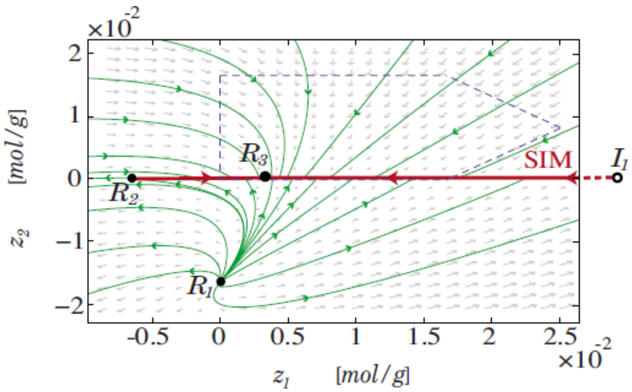
Zebrafish patterning

Bifurcations of tumor models





Nine-point problem



$H_2+O_2 \rightleftharpoons 2OH$

$OH+H_2 \rightleftharpoons H_2O+H$

$H+O_2 \rightleftharpoons OH+O$

$O+H_2 \rightleftharpoons OH+H$

$H+O_2+M \rightleftharpoons HO_2+M$ [b]

$H+2O_2 \rightleftharpoons HO_2+O_2$

$H+O_2+N_2 \rightleftharpoons HO_2+N_2$

$OH+HO_2 \rightleftharpoons H_2O+O_2$

$H+HO_2 \rightleftharpoons 2OH$

$O+HO_2 \rightleftharpoons O_2+OH$

$2OH \rightleftharpoons O+H_2O$

$H_2+M \rightleftharpoons 2H+M$ [c]

$O_2+M \rightleftharpoons 2O+M$

$H+OH+M \rightleftharpoons H_2O+M$ [d]

$H+HO_2 \rightleftharpoons H_2+O_2$

$2HO_2 \rightleftharpoons H_2O_2+O_2$

$H_2O_2+M \rightleftharpoons 2OH+M$

$H_2O_2+H \rightleftharpoons HO_2+H_2$

$H_2O_2+OH \rightleftharpoons H_2O+HO_2$

Chemical reactions

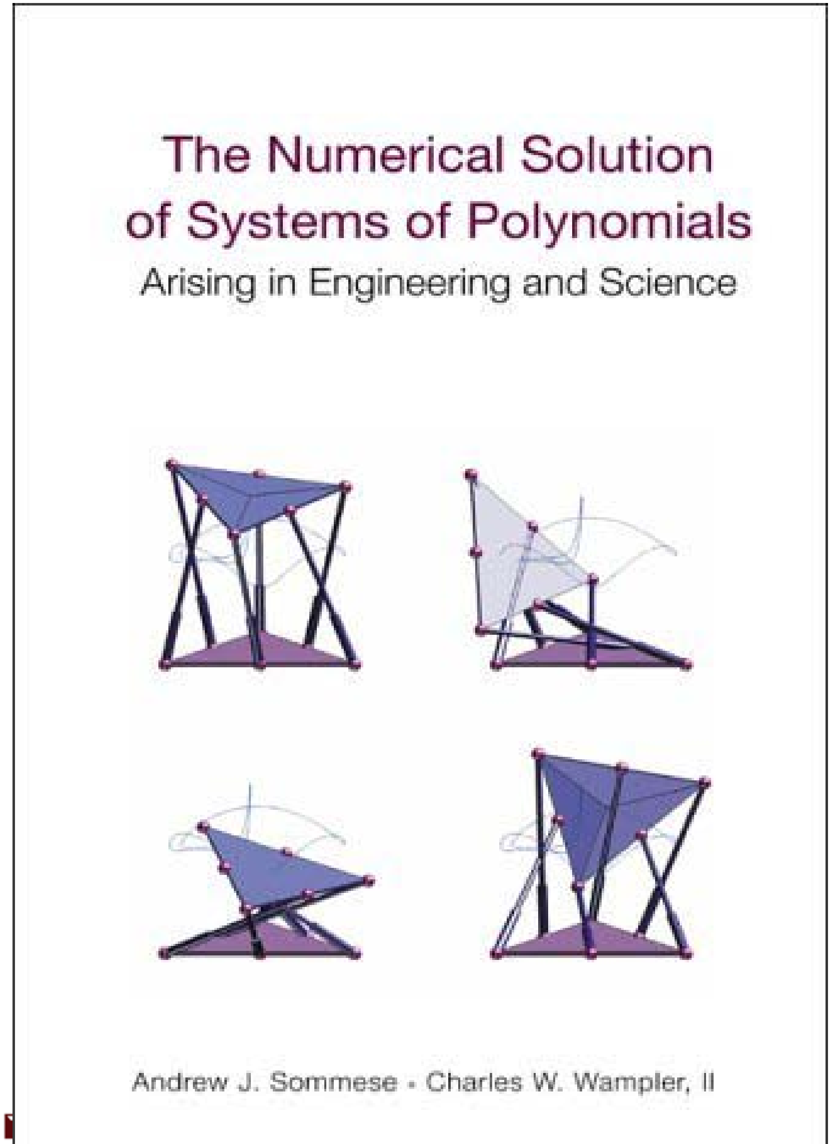
Overview

- Homotopy continuation
- Basic numerical algebraic geometry
- Regeneration
- Rank-deficiency sets

Joint work with

- D. Bates (Colorado State)
- C. Peterson (Colorado State)
- A. Sommese (Notre Dame)
- C. Wampler (General Motors R&D)

General references



T.Y. Li, Numerical solution of polynomial systems by homotopy continuation methods, in *Handbook of Numerical Analysis*, Volume XI, 209–304, North-Holland, 2003.

General references

D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler,
Bertini: Software for Numerical Algebraic Geometry.
Available at www.nd.edu/∼sommese/bertini.

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Homotopy continuation

Main problem in numerical algebraic geometry:
Describe all $x \in \mathbb{C}^N$ where

$$f(x) = \begin{bmatrix} f_1(x_1, \ldots, x_N) \\ \vdots \\ f_n(x_1, \ldots, x_N) \end{bmatrix} = 0$$

and each f_i is polynomial.

Homotopy continuation

Basic isolated root finding:
Assume $n = N$ ("square"). Compute the isolated solutions of

$$f(x) = \begin{bmatrix} f_1(x_1, \ldots, x_N) \\ \vdots \\ f_n(x_1, \ldots, x_N) \end{bmatrix} = 0.$$

Homotopy continuation

Algorithm

- Treat f as a member of a parameterized family of polynomial systems $\mathcal{F}$.
- Compute the isolated roots of $g \in \mathcal{F}$ (general enough).
- Setup the homotopy $H(x, t) = (1 - t)f(x) + tg(x)$.
- Track the paths $x(t)$ defined by $H(x(t), t) \equiv 0$.
  Since $H(x(1), 1) = g(x(1)) = 0$, paths start at the known roots of g.

Homotopy continuation

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  Since $H(x(1),1) = g(x(1)) = 0$, paths start at the known roots of g.

Computing the roots of g is very interesting when nontrivial.

B. Huber and B. Sturmfels, A polyhedral method for solving sparse polynomial systems, *Math. Comp.* 64(212), 1541–1555, 1995.

Homotopy continuation

Example

$$f = \begin{bmatrix} x^2 + 2x - 8 \\ xy + 2x + 4y - 3 \end{bmatrix}$$

1. Total degree: $\mathcal{F} = \left\{ \begin{bmatrix} g_1(x,y) \\ g_2(x,y) \end{bmatrix} : \deg(g_i) = 2 \right\}$,

$$g = \begin{bmatrix} x^2 - 1 \\ y^2 - 1 \end{bmatrix}, \text{ Bound: } 4.$$

Homotopy continuation

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   $$g = \begin{bmatrix} x^2 - 1 \\ y^2 - 1 \end{bmatrix},\ \text{Bound: } 4.$$

2. 2-hom: $\mathcal{F} = \left\{ \begin{bmatrix} g_1(x) \\ g_2(x,y) \end{bmatrix} : \begin{array}{l} \deg(g_1) = 2 \\ \deg_x(g_2) = \deg_y(g_2) = 1 \end{array} \right\}$,

   $$g = \begin{bmatrix} x^2 - 1 \\ (x-2)(y-1) \end{bmatrix},\ \text{Bound: } 2.$$

Homotopy continuation

Example

$$f = \begin{bmatrix} x^2 + 2x - 8 \\ xy + 2x + 4y - 3 \end{bmatrix}$$

3. Polytope: $\mathcal{F} = \left\{ \begin{bmatrix} a_1 x^2 + a_2 x + a_3 \\ a_4 xy + a_5 x + a_6 y + a_7 \end{bmatrix} : a_i \in \mathbb{C} \right\}$,

$$g = \begin{bmatrix} x^2 - 1 \\ y - 1 \end{bmatrix},$$ Bound: 2.

Homotopy continuation

Example

$$f = \begin{bmatrix} x^2 + 2x - 8 \\ xy + 2x + 4y - 3 \end{bmatrix}$$

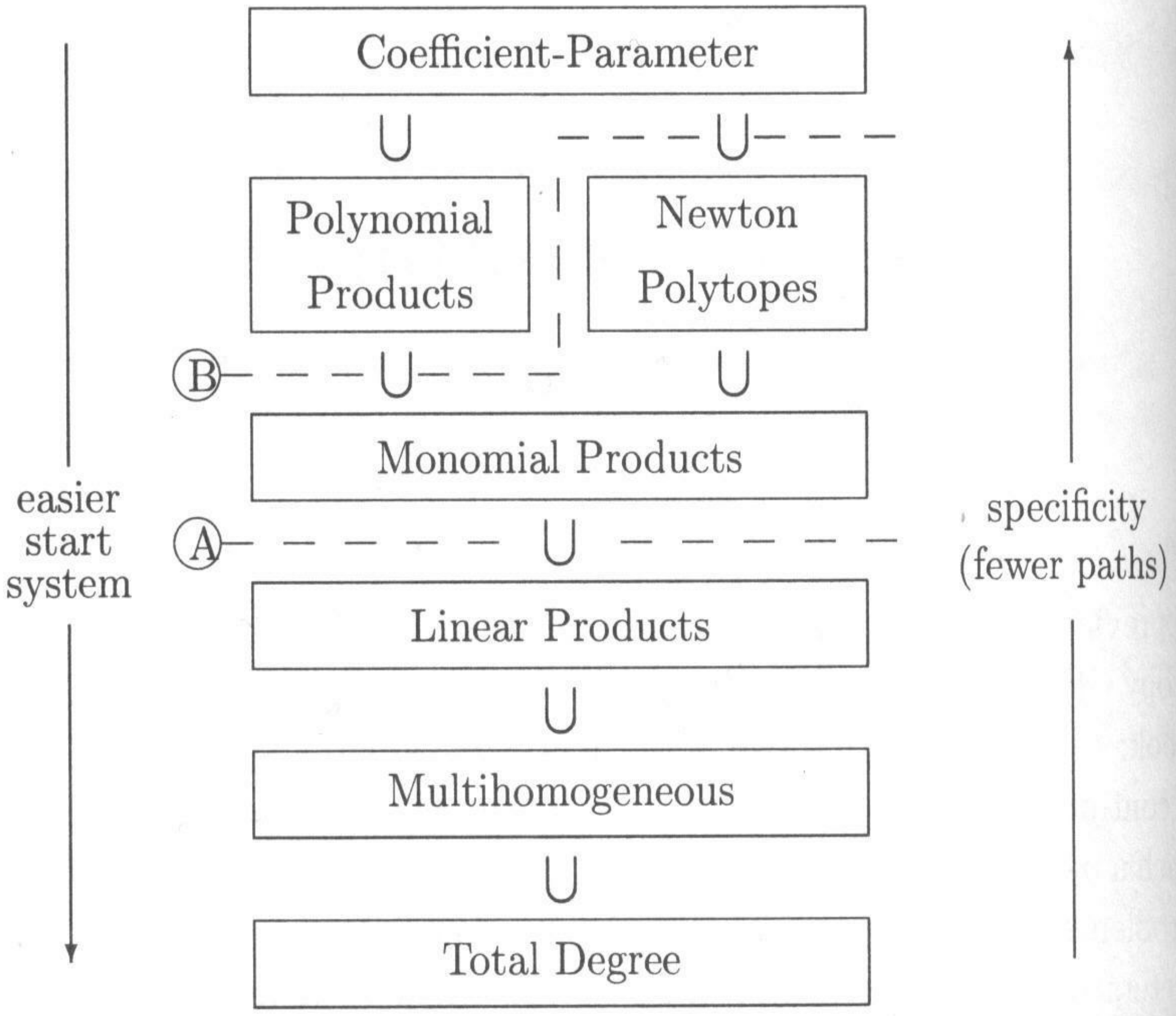
3. Polytope: $\mathcal{F} = \left\{ \begin{bmatrix} a_1 x^2 + a_2 x + a_3 \\ a_4 xy + a_5 x + a_6 y + a_7 \end{bmatrix} : a_i \in \mathbb{C} \right\}$,

   $g = \begin{bmatrix} x^2 - 1 \\ y - 1 \end{bmatrix}$, Bound: 2.

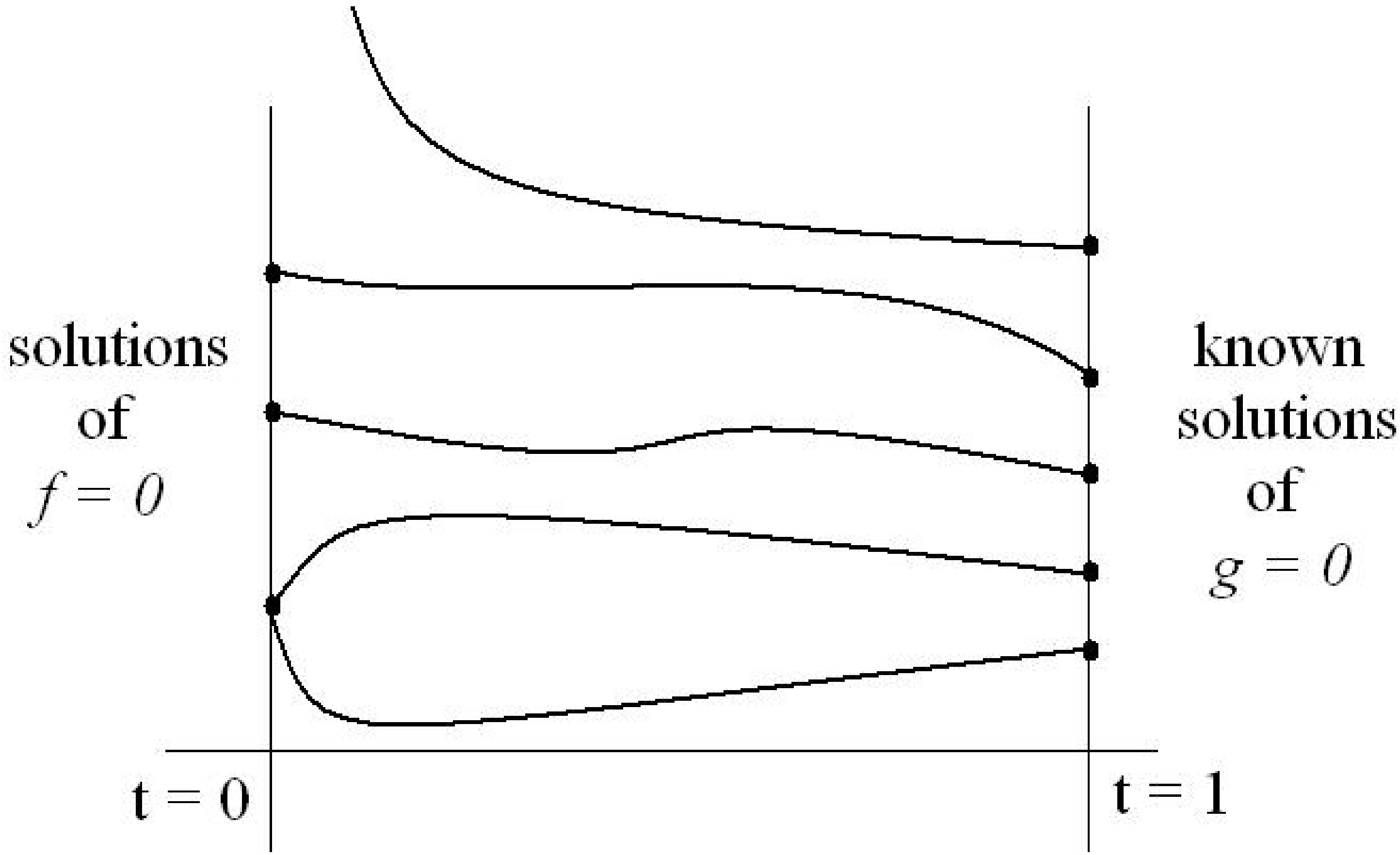
4. "Optimal": $\mathcal{F} = \left\{ \begin{bmatrix} x^2 - (a_1 + a_2)x + a_1 a_2 \\ (x - a_1)y + a_3 x + a_4 \end{bmatrix} : a_i \in \mathbb{C} \right\}$,

   $g = \begin{bmatrix} x^2 - 1 \\ (x+1)y - 2 \end{bmatrix}$, Bound: 1.

Homotopy continuation



Homotopy continuation



$$H(x,t) = (1-t)f(x) + tg(x) \equiv 0$$

Homotopy continuation

For a properly constructed homotopy:

- Solution paths $x(t)$ exist
- Solution paths $x(t)$ satisfy the Davidenko differential equation

$$0 \equiv \frac{dH(x(t),t)}{dt} = \frac{\partial H(x(t),t)}{\partial x} x'(t) + \frac{\partial H(x(t),t)}{\partial t}.$$

- For $t \neq 0$, $\frac{\partial H(x(t),t)}{\partial x}$ is invertible.
- $\{\text{isolated roots of } f\} \subset$
  $\{x(0) = \lim_{t \to 0} x(t) \mid x(1) \text{ is an isolated root of } g\}$

Homotopy continuation

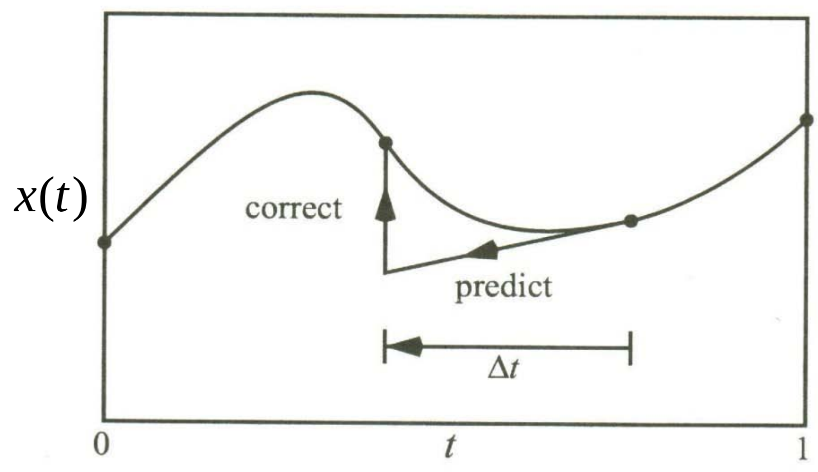
Track solution paths using a predictor-corrector scheme.

Predict using Davidenko's differential equation:

$$\frac{\partial H(x(t),t)}{\partial x}x'(t) = -\frac{\partial H(x(t),t)}{\partial t}.$$

Correct using Newton's method:

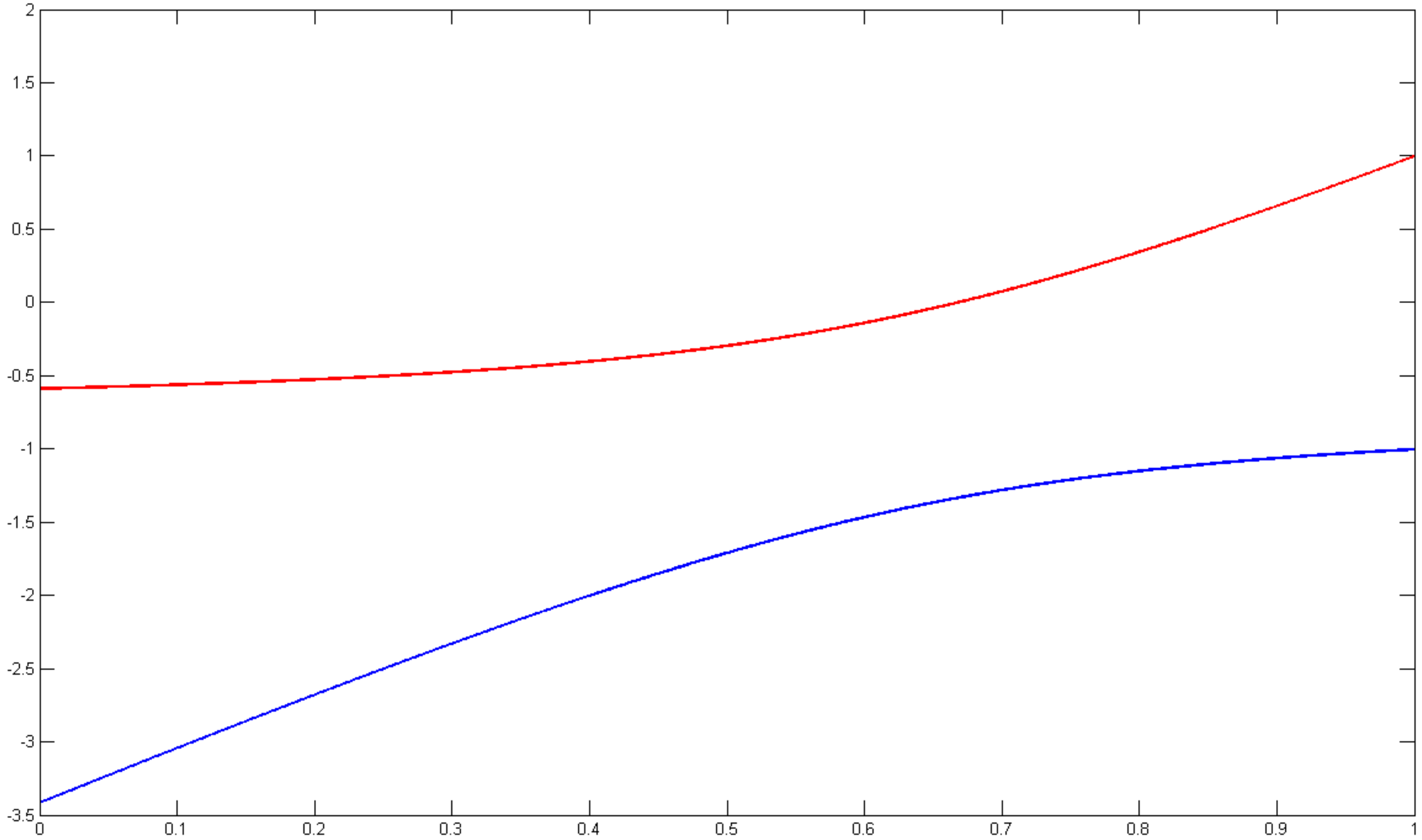
$$H(x(t),t) \equiv 0.$$



Example

$f(x) = x^2 + 4x + 2$

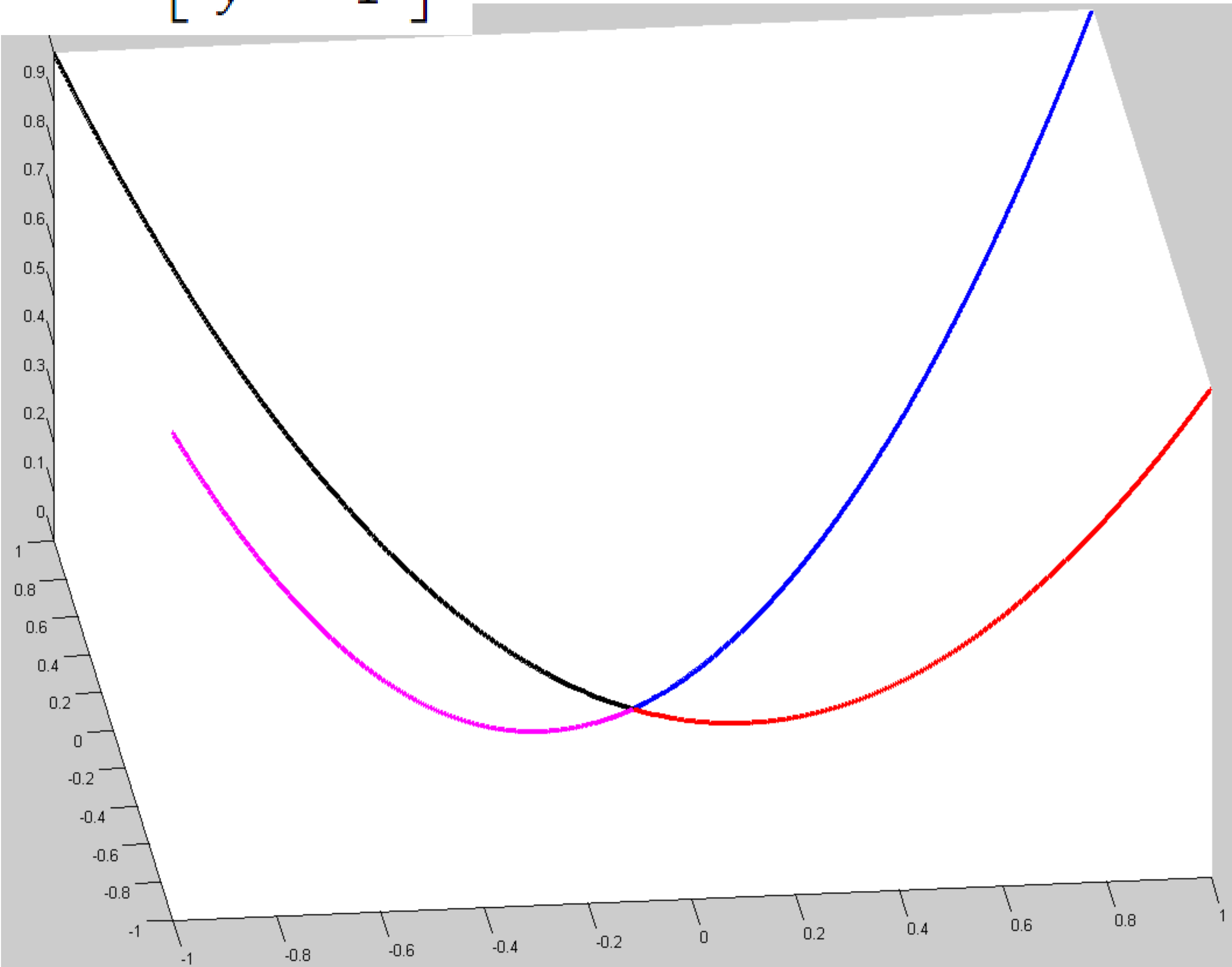
$H(x, t) = (1 - t)f(x) + t(x^2 - 1).$



Example

$$f(x,y) = \begin{bmatrix} x^2 \\ y^2 \end{bmatrix}$$

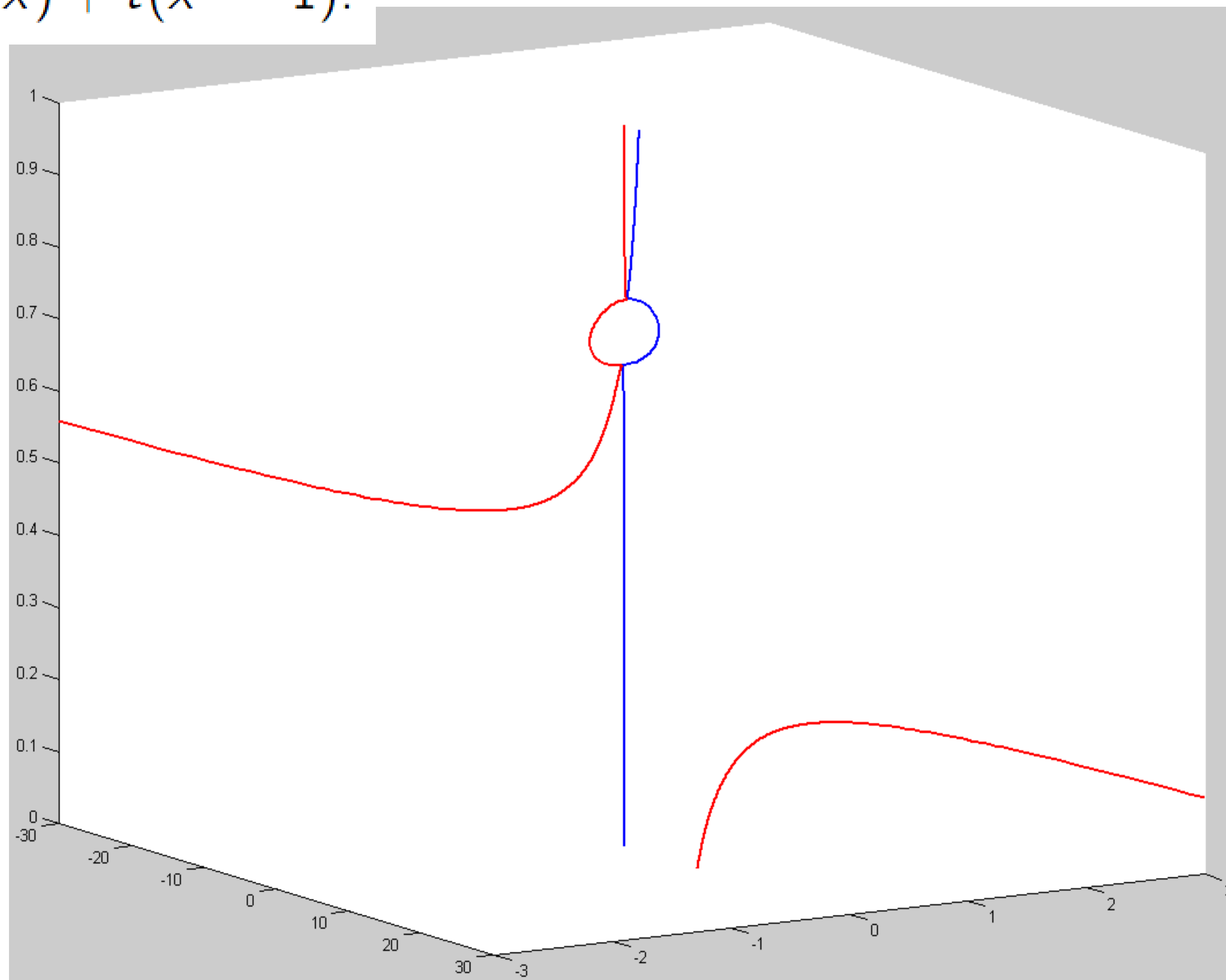
$$H(x,y,t) = (1-t)f(x,y) + t\begin{bmatrix} x^2 - 1 \\ y^2 - 1 \end{bmatrix}.$$



Example

$$f(x) = -\frac{1}{2}x^2 + 4x + \frac{14}{3}$$

$$H(x,t) = (1-t)f(x) + t(x^2-1).$$

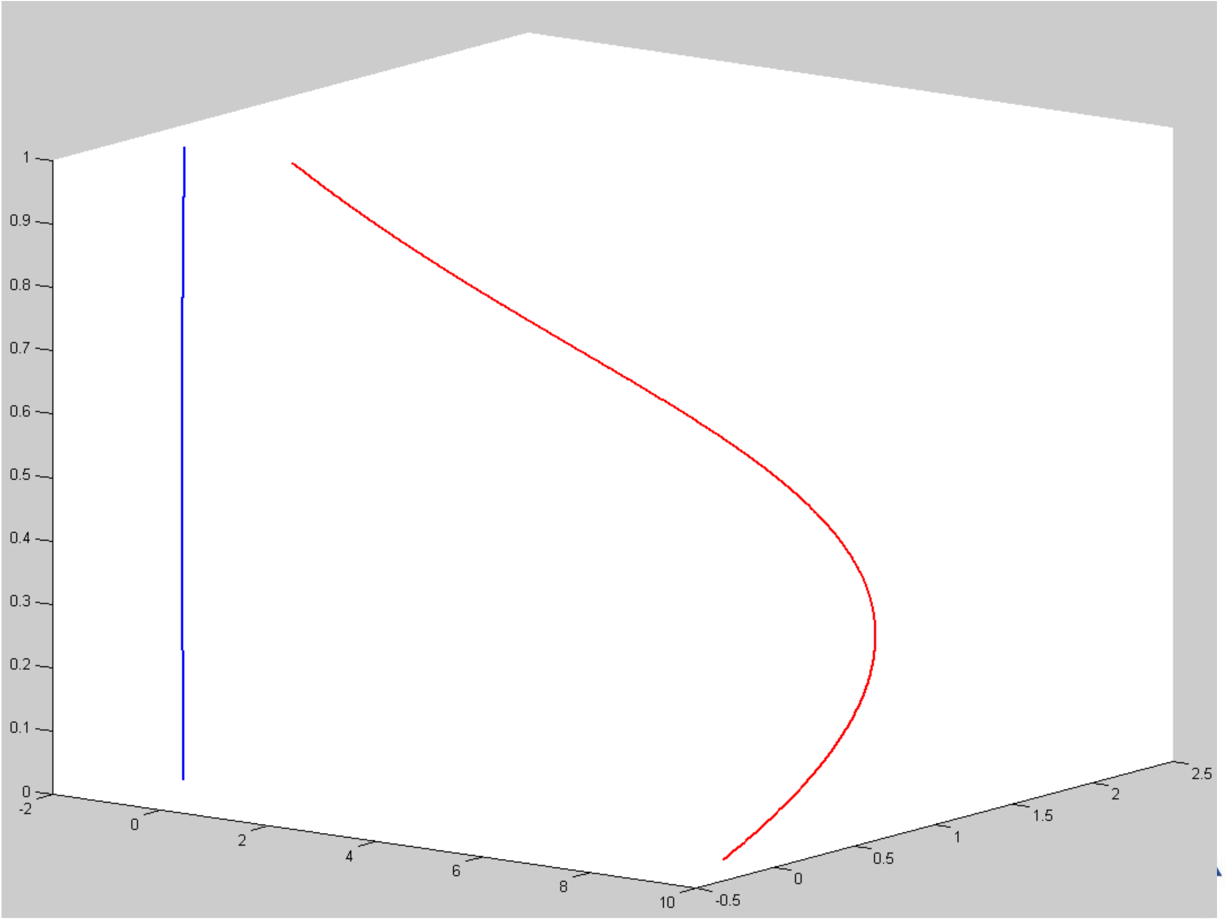


Example

$f(x) = -\frac{1}{2}x^2 + 4x + \frac{14}{3}$

For random $\gamma \in \mathbb{C}$,

$H(x,t) = (1-t)f(x) + \gamma t(x^2 - 1)$.



Homotopy continuation

Singular endpoints occur frequently.

- Endgames: compute the endpoint by staying sufficiently far away from $t = 0$.
- Deflation: restore quadratic convergence of Newton iterations.

Example

$$f = \begin{bmatrix} x^2 \\ y^2 \end{bmatrix} \quad H = \begin{bmatrix} x^2 - t \\ y^2 - t \end{bmatrix}$$

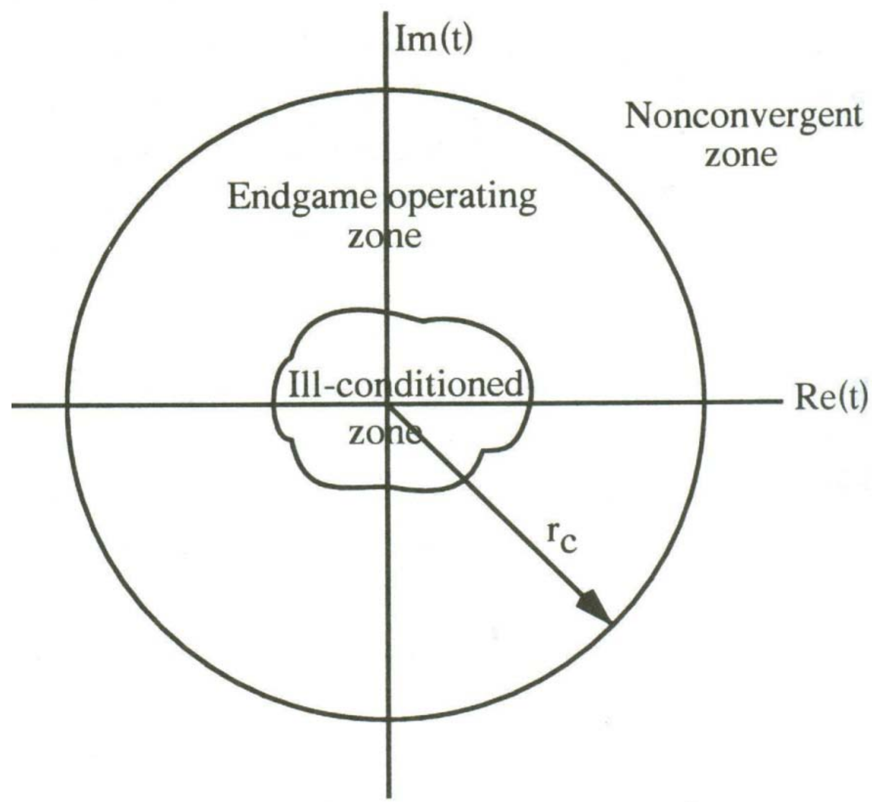
$$J = \begin{bmatrix} 2x & 0 \\ 0 & 2y \end{bmatrix}.$$

$$J \rightarrow 0 \text{ as } t \rightarrow 0.$$

Homotopy continuation

Endgame algorithms accurately compute the endpoint of the path by using the local Puiseux series expansion:

$$x(t) = x(0) + \sum_{j \geq 1} a_j t^{j/c}.$$



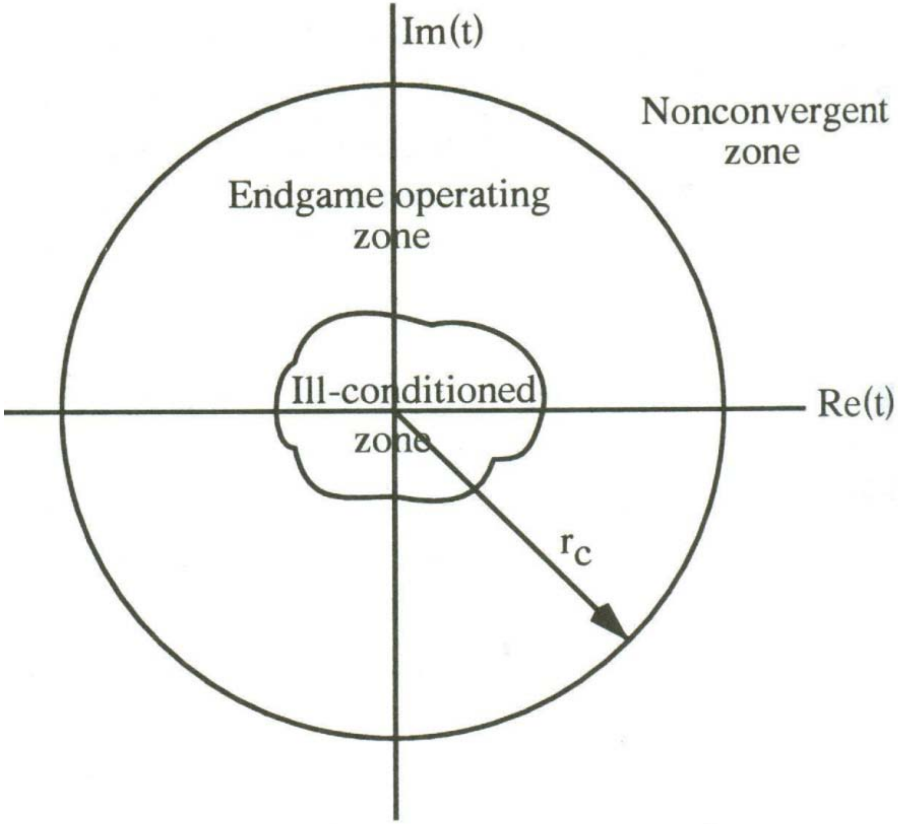
Use high enough precision to ensure reliable numerical computations.

Homotopy continuation

$$x(t) = x(0) + \sum_{j \geq 1} a_j t^{j/c}$$

Cauchy integral theorem:

$$x(0) = \frac{1}{2\pi c} \int_0^{2\pi c} x(Re^{i\theta}) d\theta.$$



Homotopy continuation

Deflation for isolated solutions

A. Leykin, J. Verschelde, and A. Zhao, Newton's method with deflation for isolated singularities of polynomial systems, *Theor. Comput. Sci.*, 359, 111–122, 2006.

$$\begin{bmatrix} x^2 \\ y^2 \end{bmatrix} \quad \Longrightarrow \quad \begin{bmatrix} x^2 \\ y^2 \\ 2x\lambda_1 \\ 2y\lambda_2 \\ \alpha_1\lambda_1 + \alpha_2\lambda_2 - 1 \\ \beta_1\lambda_1 + \beta_2\lambda_2 - 1 \end{bmatrix}$$

$$(0,0), \mathrm{mult}\ 4 \qquad \left(0, 0, \widehat{\lambda_1}, \widehat{\lambda_2}\right), \mathrm{mult}\ 1$$

Homotopy continuation

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- For $t \neq 0$, $\frac{\partial H(x(t),t)}{\partial x}$ is invertible.
- {isolated roots of f} $\subset$

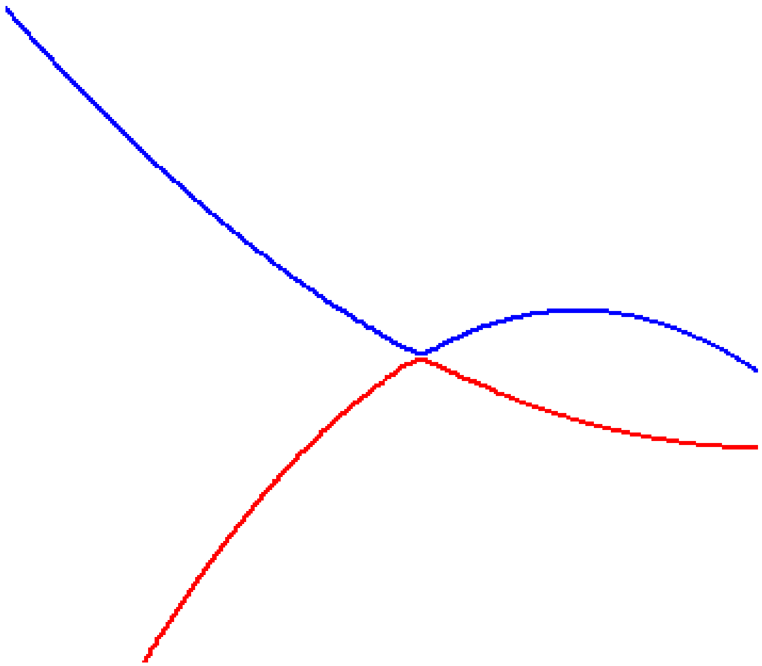
$$\{x(0) = \lim_{t\to 0} x(t) \mid x(1) \text{ is an isolated root of } g\}$$

Homotopy continuation

Near singularities arise often that can make path tracking numerically challenging.

D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler, Adaptive multiprecision path tracking. *SIAM J. Num. Anal.*, 46(2), 722–746, 2008.

D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler, Stepsize control for adaptive multiprecision path tracking. *Contemp. Math.*, 496, 21–31, 2009.



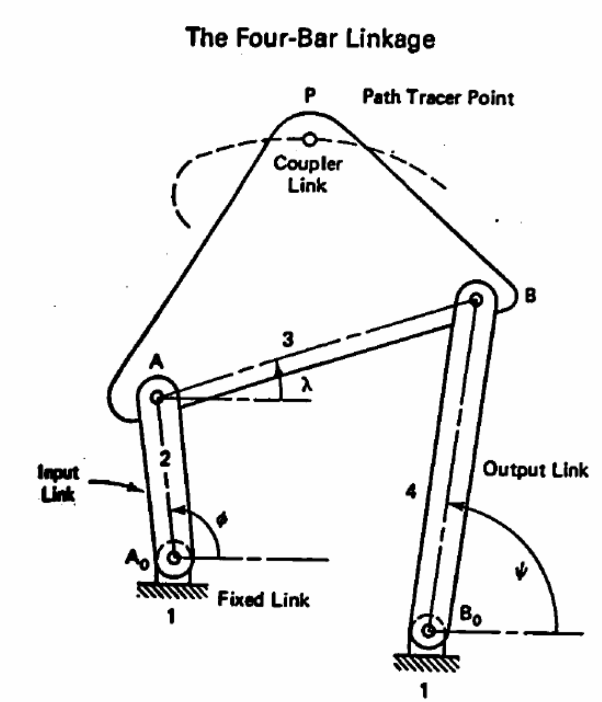
Homotopy continuation

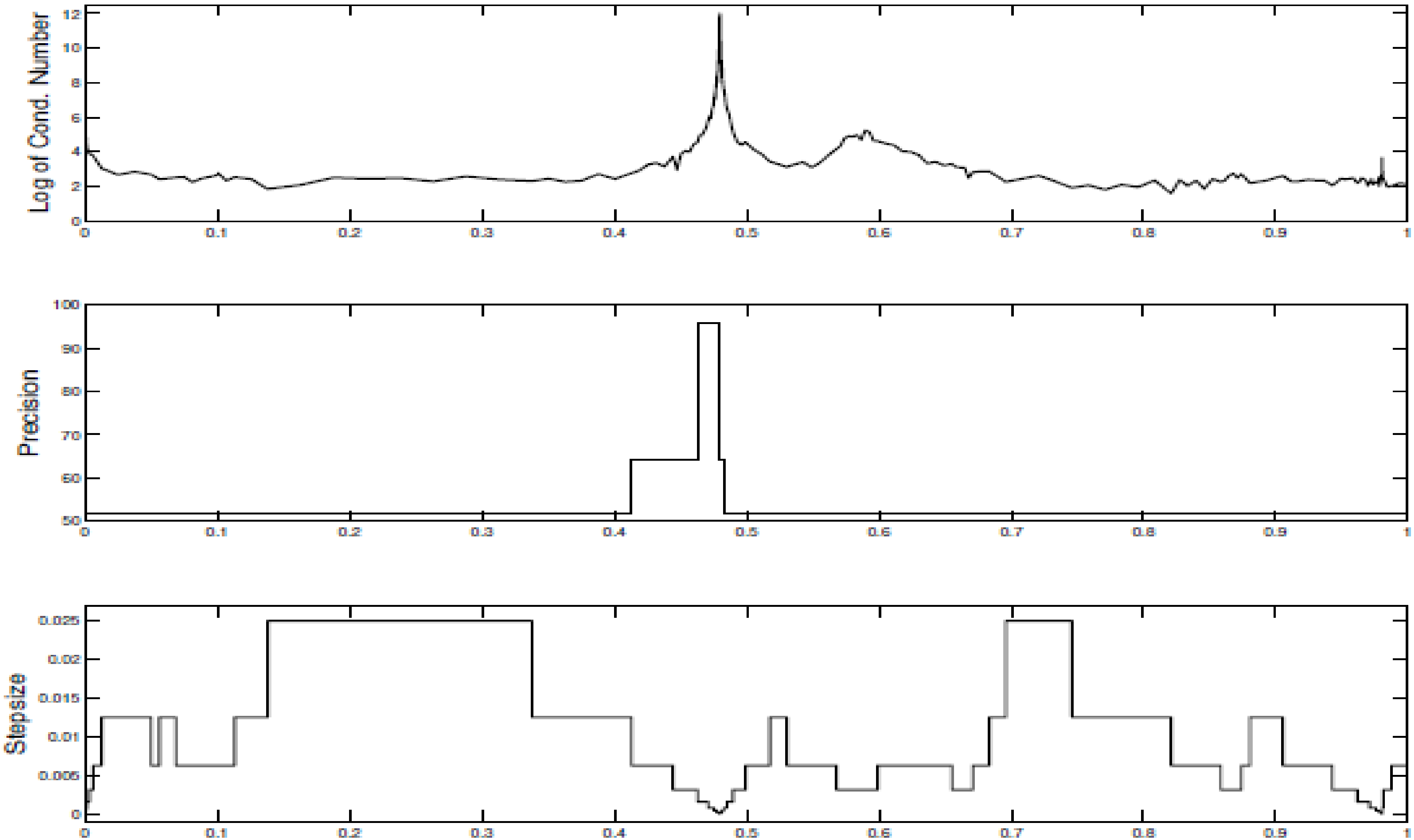
Applied the method of

D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler, Stepsize control for adaptive multiprecision path tracking. *Contemp. Math.*, 496, 21–31, 2009.

to the nine-point problem for four-bar linkages.

Out of 143,360 paths,
1184 paths (0.83%) needed higher precision to successfully track past near-singularity conditions.





D.J. Bates, J.D. Hauenstein, A.J. Sommese, and C.W. Wampler, Stepsize control for adaptive multiprecision path tracking. *Contemp. Math.*, 496, 21–31, 2009.

Homotopy continuation

Using only double precision is fast, but can lead to path crossings

T.L. Lee, T.Y. Li, C.H. Tsai, HOM4PS-2.0: a software package for solving polynomial systems by the polyhedral homotopy continuation method. *Computing*, 83(2-3), 109–133, 2008.

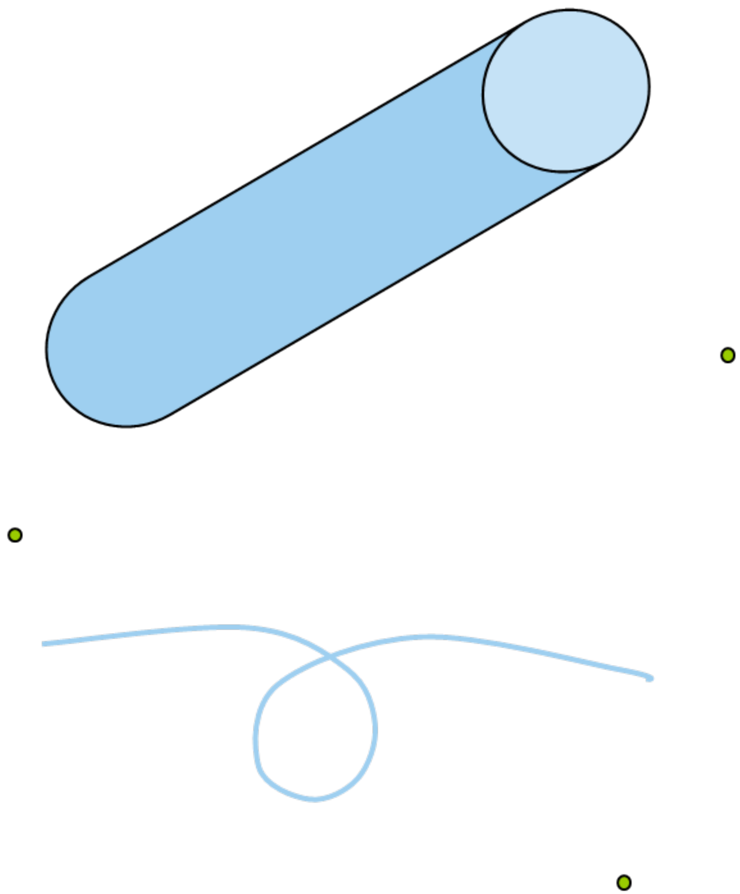
and results may not be correct.

H. Tari, H.J. Su, and T.Y. Li, A constrained homotopy technique for excluding unwanted solutions from polynomial equations arising in kinematics problems. To appear in *Mechanism and Machine Theory*.

Numerical algebraic geometry

Positive-dimensional solution sets can be handled by intersecting with random linear spaces to reduce down to the isolated case.

A.J. Sommese and C.W. Wampler, Numerical algebraic geometry. *The mathematics of numerical analysis* (Park City, UT 1995). Vol. 32 of *Lectures in Appl. Math.*, 749–763, AMS, Providence, RI, 1996.



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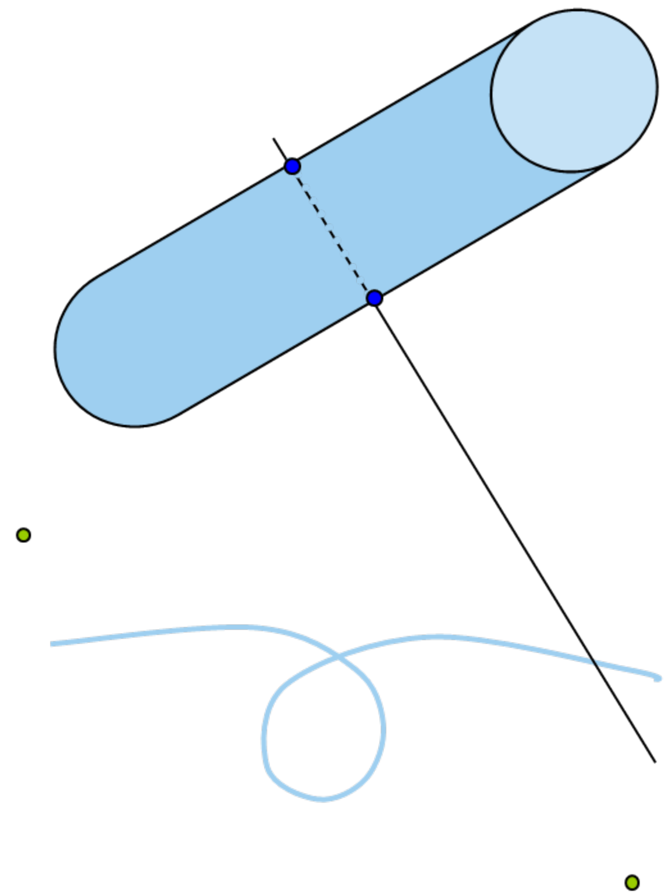

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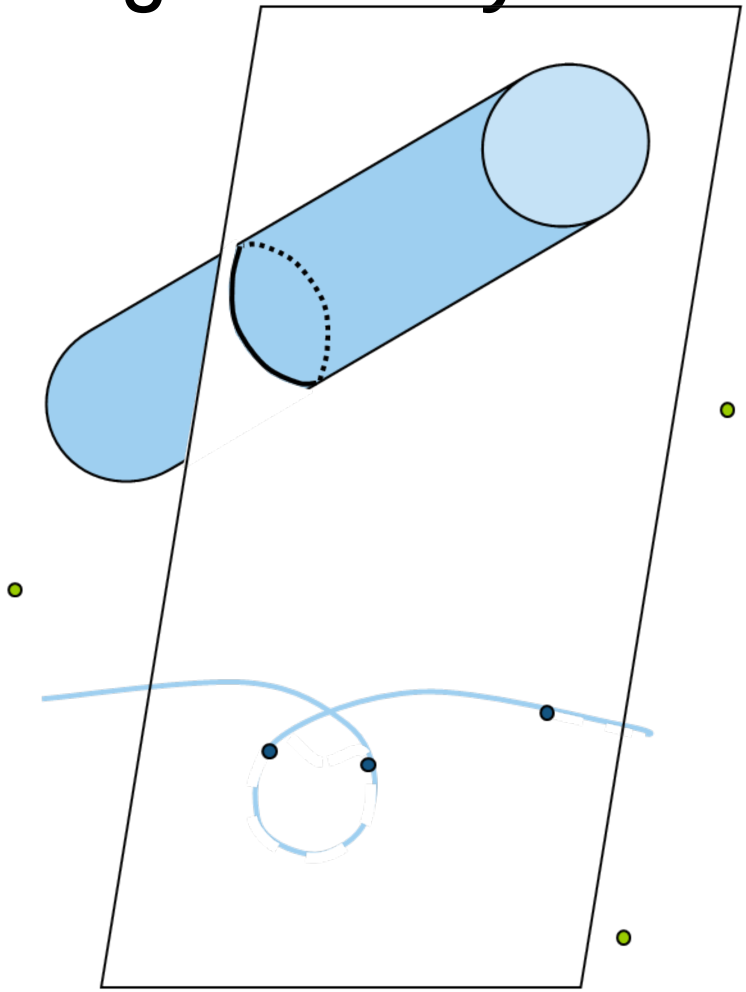
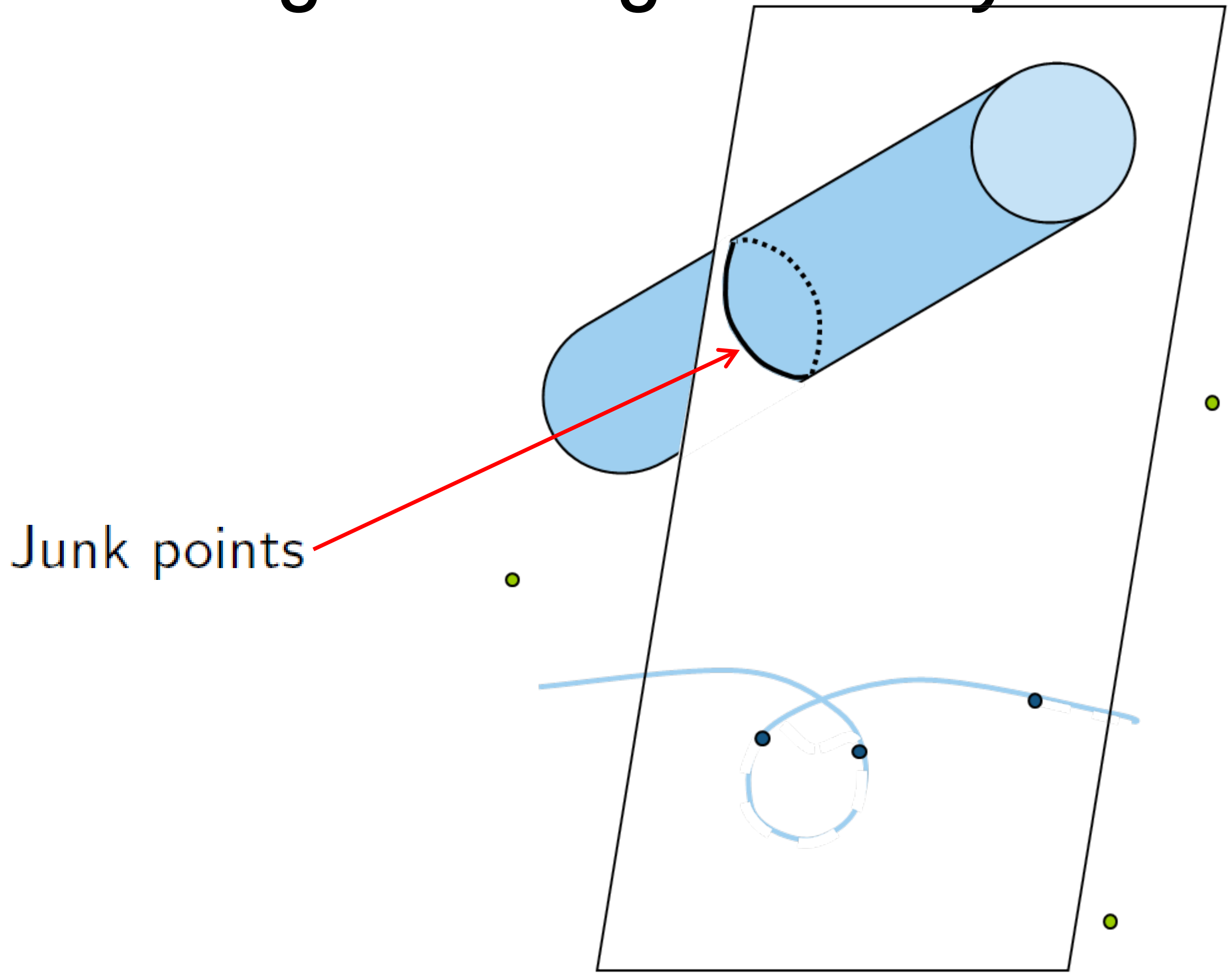


A.J. Sommese and C.W. Wampler, Numerical algebraic geometry. *The mathematics of numerical analysis* (Park City, UT 1995). Vol. 32 of *Lectures in Appl. Math.*, 749–763, AMS, Providence, RI, 1996.

Numerical algebraic geometry

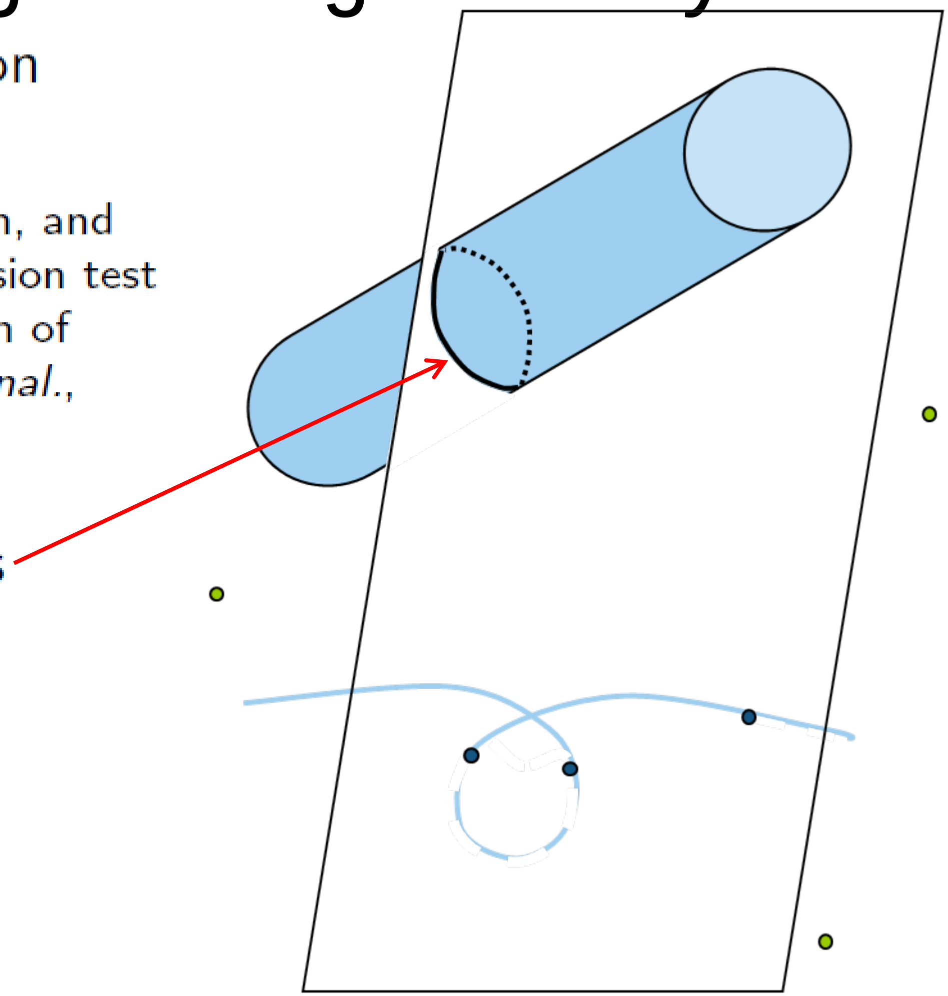


Numerical algebraic geometry

Compute a local Hilbert function to determine if isolated.

D.J. Bates, J.D. Hauenstein, C. Peterson, and A.J. Sommese, A numerical local dimension test for points on the solution set of a system of polynomial equations. *SIAM J. Num. Anal.*, 47(5), 3608–3623, 2009.

Junk points



Numerical algebraic geometry

Numerical irreducible decomposition algorithm:

1. Compute a *witness superset* $\widehat{W}_k$ for each dimension k.
   - Compute a superset of the isolated roots of $\begin{bmatrix} f \\ \mathcal{L}_k \end{bmatrix}$.
2. Compute a *witness set* W_k for each k.
   - Remove the nonisolated roots of $\begin{bmatrix} f \\ \mathcal{L}_k \end{bmatrix}$ from $\widehat{W}_k$.
3. Partition W_k into sets corresponding to the irreducible components of dimension k.

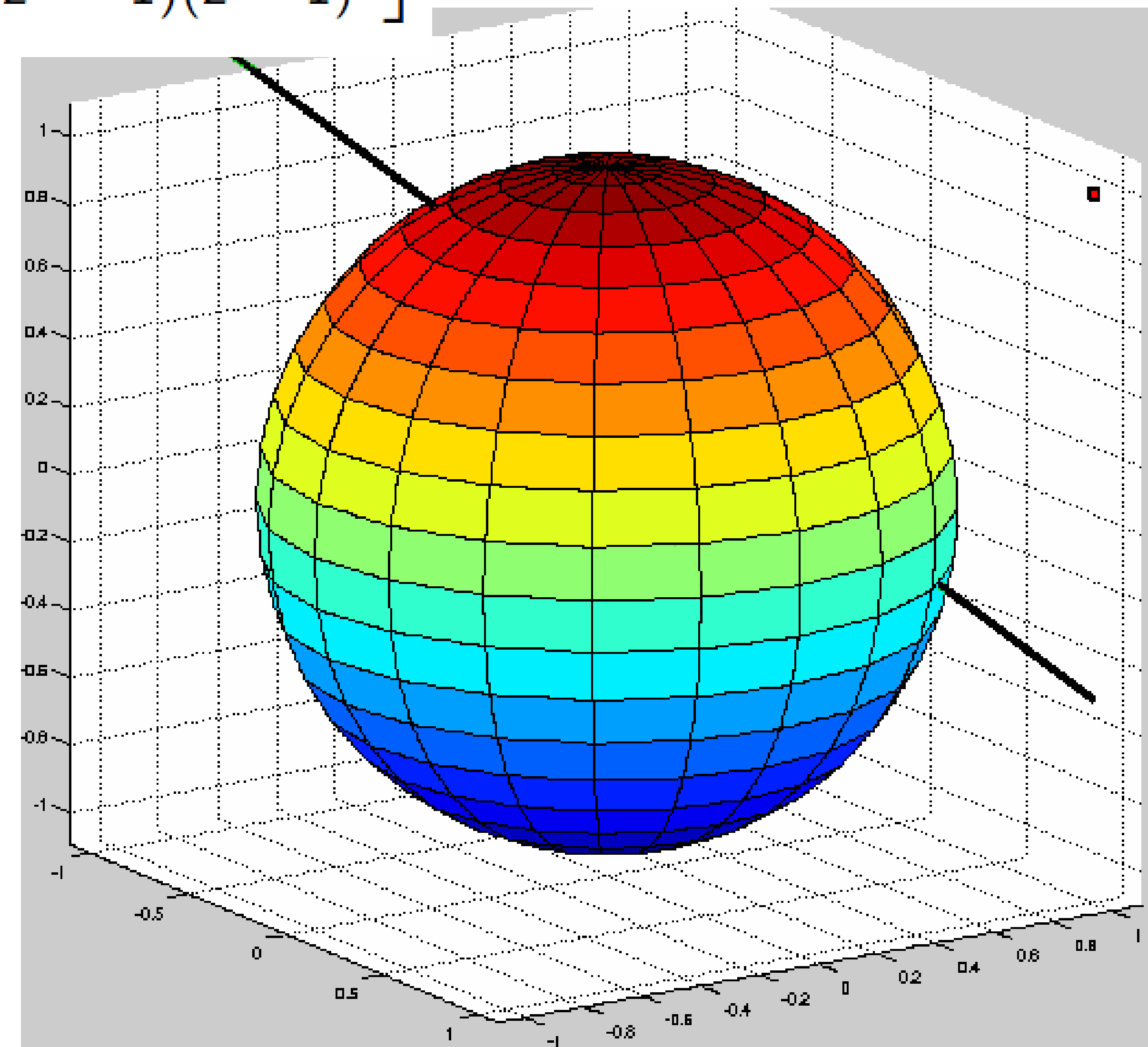
Numerical algebraic geometry

Extension of numerical irreducible decomposition to numerical primary decomposition:

A. Leykin, Numerical primary decomposition. *ISSAC 2008*, 165–172, ACM, New York, 2008.

Example

$$f(x,y,z) = \begin{bmatrix} (x^2+y^2+z^2-1)(x-1) \\ (x^2+y^2+z^2-1)(y-1) \\ (x^2+y^2+z^2-1)(z-1) \end{bmatrix}$$



Numerical algebraic geometry

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Dimension 2:

Let L_1, L_2 be random linear polynomials. Solve $\begin{bmatrix} f \\ L_1 \\ L_2 \end{bmatrix} = 0.$

$g_2 = \begin{bmatrix} f_1 + \alpha_2 f_2 + \alpha_3 f_3 \\ L_1 \\ L_2 \end{bmatrix}$ has 2 nonsingular roots that satisfy $f = 0$.

Numerical algebraic geometry

Example

$$f(x,y,z) = \begin{bmatrix} (x^2+y^2+z^2-1)(x-1) \\ (x^2+y^2+z^2-1)(y-1) \\ (x^2+y^2+z^2-1)(z-1) \end{bmatrix}$$

Dimension 1:

Solve $\begin{bmatrix} f \\ L_1 \end{bmatrix} = 0.$

$g_1 = \begin{bmatrix} f_1 + \alpha_2 f_2 + \alpha_3 f_3 \\ f_2 + \beta_3 f_3 \\ L_1 \end{bmatrix}$ has 8 singular roots that

satisfy $f = 0$ - all are junk points.

Numerical algebraic geometry

Example

$$f(x,y,z) = \begin{bmatrix} (x^2+y^2+z^2-1)(x-1) \\ (x^2+y^2+z^2-1)(y-1) \\ (x^2+y^2+z^2-1)(z-1) \end{bmatrix}$$

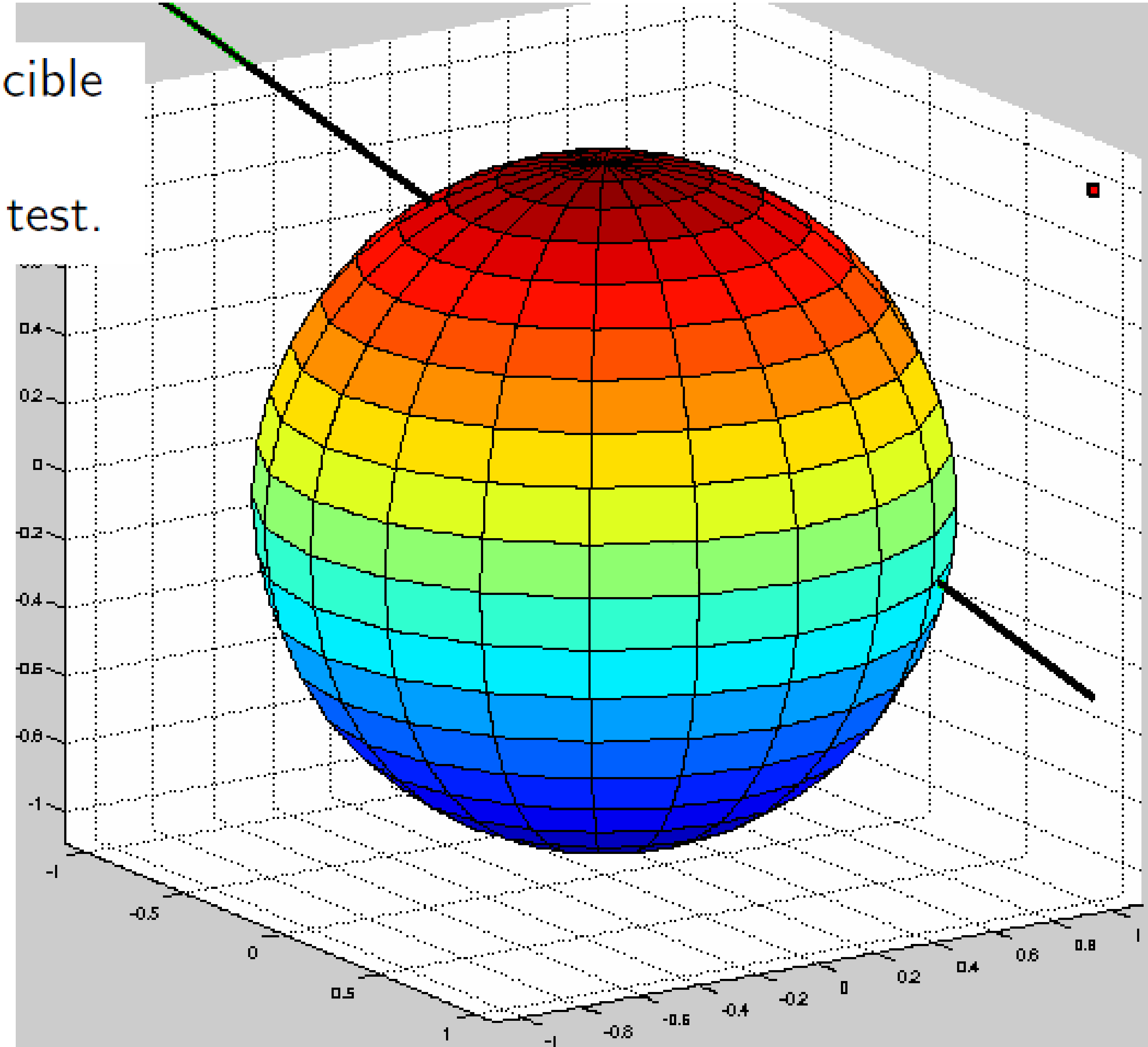
Dimension 0:

Solve $f = 0$.

1 nonsingular root and 26 singular roots - all are junk points.

Numerical algebraic geometry

Decompose into irreducible components by using monodromy and trace test.



Numerical algebraic geometry

Bertini:

```
*************** Decomposition by Degree ***************

Dimension 2: 1 classified component
-----------------------------------------------------------
   degree 2: 1 component

Dimension 0: 1 classified component
-----------------------------------------------------------
   degree 1: 1 component

***********************************************************
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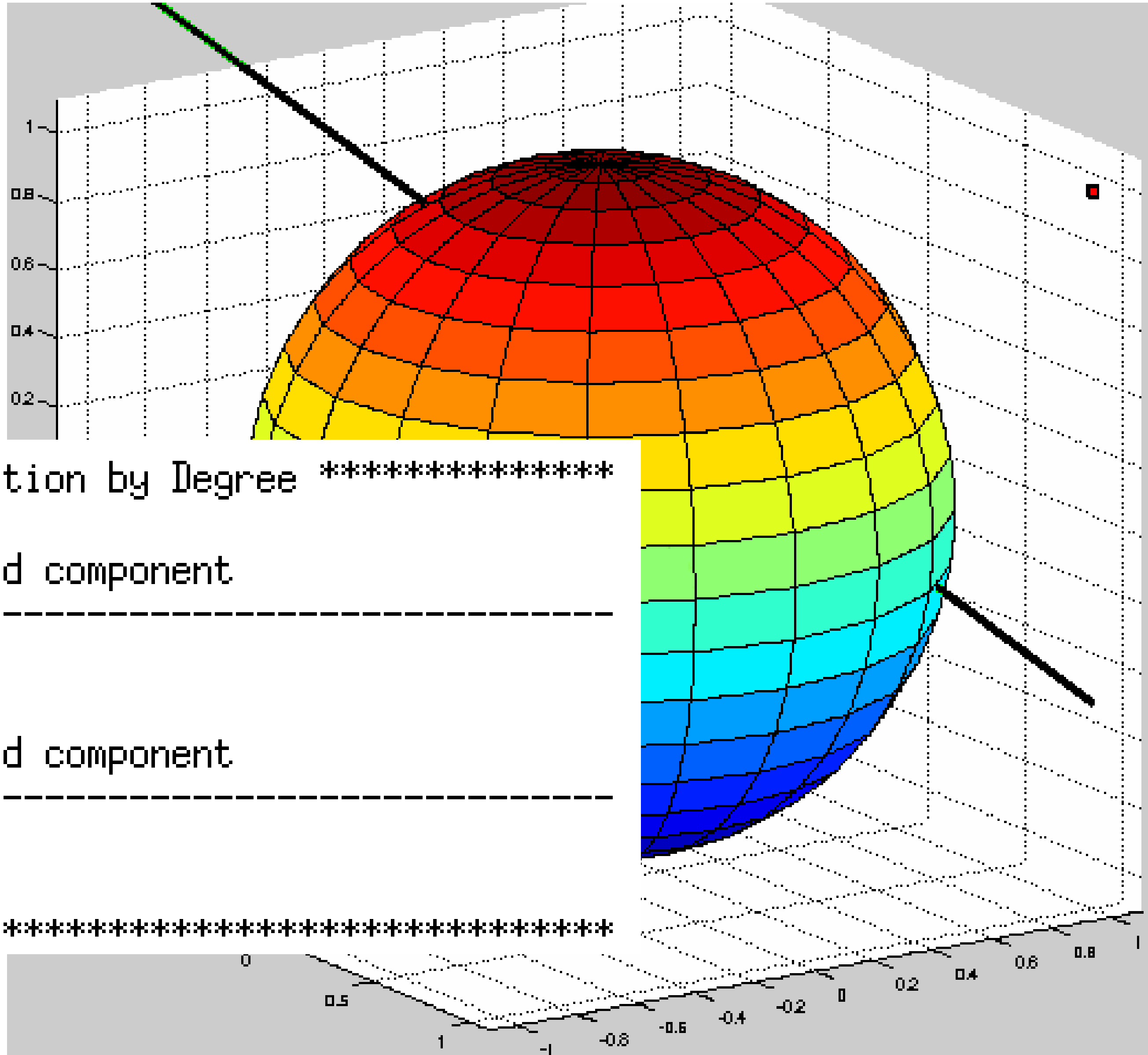

Regeneration

Given the roots of $\begin{bmatrix} f_1 \\ \vdots \\ f_k \\ L_{k+1} \\ L_{k+2} \\ \vdots \\ L_n \end{bmatrix}$, regeneration computes the roots of $\begin{bmatrix} f_1 \\ \vdots \\ f_k \\ f_{k+1} \\ L_{k+2} \\ \vdots \\ L_n \end{bmatrix}$.

J.D. Hauenstein, A.J. Sommese, and C.W. Wampler, Regeneration homotopies for solving systems of polynomials. To appear in *Mathematics of Computation*.

Regeneration

Regeneration is effective at computing nonsingular isolated solutions of large scale structured polynomial systems arising in many applications.

The *regenerative cascade* algorithm applies regeneration to

$$\mathfrak{R}(f) = \begin{bmatrix} f_1 + \alpha_{1,2} f_2 + \alpha_{1,3} f_3 + \cdots + \alpha_{1,n} f_n \\ f_2 + \alpha_{2,3} f_3 + \cdots + \alpha_{2,n} f_n \\ \vdots \\ f_n \end{bmatrix}$$

in order to compute witness supersets of f.

Regeneration

Step 1:

Move L_{k+1} to $\mathfrak{L}_1, \ldots, \mathfrak{L}_{\deg f_{k+1}}$ using

$$H_i(x,t) = \begin{bmatrix} f_1 \\ \vdots \\ f_k \\ \mathfrak{L}_i(1-t) + tL_{k+1} \\ L_{k+2} \\ \vdots \\ L_n \end{bmatrix}.$$

Regeneration

Step 2:

Introduce f_{k+1} using

$$H(x,t) = \begin{bmatrix} f_1 \\ \vdots \\ f_k \\ f_{k+1}(1-t) + t\prod_{i=1}^{\deg f_{k+1}} \mathfrak{L}_i \\ L_{k+2} \\ \vdots \\ L_n \end{bmatrix}.$$

Regeneration

Adjacent minor system:

> Determinants of 2×2 adjacent minors of $3 \times n$ matrix with variable entries.

Regeneration

Adjacent minor system:

> Determinants of 2×2 adjacent minors of $3 \times n$ matrix with variable entries.

For example: $n = 3$

$$\begin{bmatrix} x_1 & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{bmatrix}$$

Regeneration

Adjacent minor system:

> Determinants of 2×2 adjacent minors of $3 \times n$ matrix with variable entries.

For example: $n = 3$

$$\begin{bmatrix} x_1 & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{bmatrix}$$

$$f_1 = x_1 x_5 - x_2 x_4$$

Regeneration

Adjacent minor system:

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Regeneration

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$$\left[\begin{array}{c|cc|} x_1 & x_2 & x_3 \\ x_4 & x_5 & x_6 \\ x_7 & x_8 & x_9 \end{array}\right]$$

$$f_1 = x_1x_5 - x_2x_4 \qquad f_3 = x_4x_8 - x_5x_7$$

$$f_2 = x_2x_6 - x_3x_5 \qquad f_4 = x_5x_9 - x_6x_8$$

Regeneration

Adjacent minor system:

	Membership test			Local dimension test		
n	Regen cascade	Dim-by-dim	Cascade	Regen cascade	Dim-by-dim	Cascade
3	0.1s	0.1s	0.2s	0.1s	0.1s	0.2s
4	0.8s	1.1s	1.3s	0.6s	0.8s	1.1s
5	6.2s	11.9s	11.2s	3.1s	4.6s	7.4s
6	1m1s	2m14s	1m34s	15.6s	29.0s	48.4s
7	10m36s	25m39s	14m54s	1m16s	3m8s	5m23s
8	2h12m54s	5h21m48s	2h33m5s	6m33s	19m45s	29m22s

J.D. Hauenstein, Regeneration, local dimension, and applications in numerical algebraic geometry. Ph.D. Thesis, University of Notre Dame, Notre Dame, IN, April 2009.

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Rank-deficiency sets

Given $A(x) = \begin{bmatrix} a_{1,1}(x) & \cdots & a_{1,n}(x) \\ \vdots & \ddots & \vdots \\ a_{m,1}(x) & \cdots & a_{m,n}(x) \end{bmatrix}$, compute the sets

$$S_k(A) = \{x \mid \mathrm{rank}\, A(x) \le k\} \text{ and } S_{k,f}(A) = S_k(A) \cap V(f).$$

Rank-deficiency sets

One way to compute $S_k(A)$ is by creating a polynomial system consisting of the $(k+1) \times (k+1)$ minors of A.

- Could yield impractically large system: $\binom{m}{k+1}\binom{n}{k+1}$.
- Each polynomial could consist of many terms.
- Each polynomial could be of high degree.

Rank-deficiency sets

Let $A(x) = \begin{bmatrix} a_{1,1}(x) & \cdots & a_{1,n}(x) \\ \vdots & \ddots & \vdots \\ a_{m,1}(x) & \cdots & a_{m,n}(x) \end{bmatrix}$ with $m \geq n$.

Our approach uses the fact that

$$S_k(A) = \{x \mid \mathrm{rank}\ A(x) \leq k\} = \{x \mid \mathrm{nullity}\ A(x) \geq n-k\}.$$

D.J. Bates, J.D. Hauenstein, C. Peterson, and A.J. Sommese, Numerical decomposition of the rank-deficiency set of a matrix of multivariate polynomials. *Approximate Commutative Algebra*, edited by L. Robbiano and J. Abbott, *Texts and Monographs in Symbolic Computation*, Springer, 55–77, 2009.

Rank-deficiency sets

Let $\Lambda = \begin{bmatrix} \lambda_{1,1} & \cdots & \lambda_{1,n-k} \\ \vdots & \ddots & \vdots \\ \lambda_{k,1} & \cdots & \lambda_{k,n-k} \end{bmatrix}$ and $B \in U(n)$ be random.

We want to solve

$$A(x)B \begin{bmatrix} I_{n-k} \\ \Lambda \end{bmatrix} = 0.$$

Remarks

- Added $k(n-k)$ new variables.
- Consists of $m(n-k)$ functions:
  - naturally 2-homogeneous
  - degree in x is same as in $A(x)$
  - linear in λ's
  - straight-line formulation

Rank-deficiency sets

Example

Compute $S_2(A)$ for $A = \begin{bmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{bmatrix}$.

Determinants: Solve 12 cubics on $\mathbb{C}^6$.
Nullity: Solve 8 polynomials of type $(1,1)$ on $\mathbb{C}^6 \times \mathbb{C}^4$.

$$S_2(A) = V(af + cd - be)$$

Rank-deficiency sets

Example

Compute the singular points of

$$f(x_1, x_2, x_3, x_4) = \begin{bmatrix} x_1 + x_2 + x_3 + x_4 \\ x_1x_2 + x_2x_3 + x_3x_4 + x_4x_1 \\ x_1x_2x_3 + x_2x_3x_4 + x_3x_4x_1 + x_4x_1x_2 \\ x_1x_2x_3x_4 - 1 \end{bmatrix}$$

on the irreducible component $C = \{(x_1, x_2, -x_1, -x_2) \mid x_1x_2 = 1\}$.

Rank-deficiency sets

Note that $\mathrm{rank}\ Jf = 3$ generically on C.

Starting with a witness set for C, we compute

$$S_2(Jf) \cap C = \{(1,1,-1,-1),(-1,-1,1,1),(i,-i,-i,i),(-i,i,i,-i)\}\,.$$