Computing Isolated Singular Solutions of Polynomial Systems using Newton's Method with Deflation

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Symposium in honor of Tien-Yien Li's 60th Birthday 10-12 May 2005 Joint work with Anton Leykin and Ailing Zhao.

outline

Computing Singular Isolated Roots

(Outline of the Talk)

- Problem: Newton fails for singular roots.
 Our goal is to restore quadratic convergence.
- Deflation Algorithm: add linear combinations of derivatives.
 We rely on only one tolerance to determine the rank.
- Why it works: #deflations < multiplicity.
 The deflation reduces #monomials under the staircase.
- 4. Implementation and Examples: Reconditioning.We use a directed acyclic graph of derivative operators.

Singularities are keeping us in business

numerical analysis: bifurcation points and endgames

Rall (1966); Reddien (1978); Decker-Keller-Kelley (1983);
Griewank-Osborne (1981); Hoy (1989);
Deuflard-Friedler-Kunkel (1987); Kunkel (1989, 1996);
Morgan-Sommese-Wampler (1991); Li-Wang (1993, 1994);
Govaerts (2000).

computer algebra: standard bases (SINGULAR) Mora (1982); Greuel-Pfister (1996)

numerical polynomial algebra: multiplicity structure

Möller-Stetter (1995); Mourrain (1997); Stetter-Thallinger (1998); Dayton-Zeng (2005)

deflation: Ojika-Watanabe-Mitsui (1983); Lecerf (2003)

motivation

A Motivating Example: cyclic 9-roots

The system

$$f(\mathbf{x}) = \begin{cases} f_i = \sum_{j=0}^8 \prod_{k=1}^i x_{(k+j) \mod 9} = 0, & i = 1, 2, \dots, 8\\ f_9 = x_0 x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 - 1 = 0 \end{cases}$$

has 333×18 isolated regular zeros, 164 isolated 4-fold zeros, and 6 cubic 2-dimensional irreducible solution components.

Newton's method with 64 decimal places, tolerance is 10^{-60} :

- regular : 4 iterations (quadratic convergence)
 - 4-fold : 79 iterations (> 1 step for one correct decimal place)

about 20 times slower to reach same magnitude of residual ...

motivation

Multiplicity of an Isolated Zero

An isolated zero of multiplicity m occurs in numerical analysis as a cluster of m (ill-conditioned) regular zeros.

Problem: geometrical significance for overdetermined systems? \rightarrow perturbed overdetermined system has no zeros!

Analogy with Univariate Case: z_0 is *m*-fold zero of f(x) = 0: $f(z_0) = 0, \frac{\partial f}{\partial x}(z_0) = 0, \frac{\partial^2 f}{\partial x^2}(z_0) = 0, \dots, \frac{\partial^{m-1} f}{\partial x^{m-1}}(z_0) = 0$

m = number of linearly independent polynomials annihilating z_0

The dual space D_0 at \mathbf{z}_0 is spanned by \boldsymbol{m} linear independent differentiation functionals annihilating \mathbf{z}_0 .

 D_0 is the multiplicity structure of the *m*-fold zero \mathbf{z}_0 .

motivation

A Simple Example

Consider

$$f(x,y) = \begin{cases} x^2 = 0\\ xy = 0\\ y^2 = 0 \end{cases} \quad \mathbf{z}_0 = (0,0).$$

The multiplicity of \mathbf{z}_0 is 3 because

$$D_0 = \operatorname{span}\{\partial_{00}[\mathbf{z}_0], \partial_{10}[\mathbf{z}_0], \partial_{01}[\mathbf{z}_0]\}$$

with

$$\partial_{ij}[\mathbf{z}_0] = \frac{1}{i!j!} \frac{\partial^{i+j}}{\partial x^i \partial y^j} f(\mathbf{z}_0).$$

Solving means to compute \mathbf{z}_0 *and* D_0 .

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Newton's Method for Overdetermined Systems

Singular Value Decomposition of *N*-by-*n* Jacobian matrix J_f :

 $J_f = U\Sigma V^T$, U and V are orthogonal: $U^T U = I_N, V^T V = I_n$,

and singular values $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n$ as the only nonzero elements on the diagonal of the *N*-by-*n* matrix Σ (*N* > *n*).

The condition number $\operatorname{cond}(J_f(\mathbf{z})) = \frac{\sigma_1}{\sigma_n}$. $\operatorname{Rank}(J_f(\mathbf{z})) = R \iff \Sigma = \operatorname{diag}(\sigma_1, \sigma_2, \dots, \sigma_R, 0, \dots, 0).$

At a **multiple root** \mathbf{z}_0 : Rank $(J_f(\mathbf{z}_0)) = R < n$.

Close to \mathbf{z}_0 , $\mathbf{z} \approx \mathbf{z}_0$: $\sigma_{R+1} \approx 0$, or $|\boldsymbol{\sigma_{R+1}}| < \boldsymbol{\epsilon}$, $\boldsymbol{\epsilon}$ is tolerance.

Moore-Penrose inverse: $J_f^+ = V\Sigma^+ U^T$, with $R = \text{Rank}(J_f)$, and $\Sigma^+ = \text{diag}(\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, \dots, \frac{1}{\sigma_R}, 0, \dots, 0)$. Then $\Delta \mathbf{z} = -J_f(\mathbf{z})^+ f(\mathbf{z})$ is the least squares solution. Dedieu-Shub (1999); Li-Zeng (2005)

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Newton with Deflation – Simple Example revisited

$$f(x,y) = \begin{cases} x^2 = 0 \\ xy = 0 \\ y^2 = 0 \end{cases} \quad J_f(x,y) = \begin{bmatrix} 2x & 0 \\ y & x \\ 0 & 2y \end{bmatrix} \quad \frac{\mathbf{z}_0 = (0,0), m = 3}{\operatorname{Rank}(J_f(\mathbf{z}_0)) = 0}$$

A nontrivial linear combination of the columns of $J_f(\mathbf{z}_0)$ is zero.

$$G(x, y, \lambda_1, \lambda_2) = \begin{cases} f(x, y) = 0 \\ \begin{bmatrix} 2x & 0 \\ y & x \\ 0 & 2y \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$
$$c_1 \lambda_1 + c_2 \lambda_2 = 1, \qquad \text{random } c_1, c_2 \in \mathbb{C}$$

The system $G(x, y, \lambda_1, \lambda_2) = 0$ has $(0, 0, \lambda_1^*, \lambda_2^*)$ as regular zero!

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Deflation Operator Dfl reduces to Corank One

Suppose $\operatorname{Rank}(J_f(\mathbf{z}_0)) = \mathbb{R}$ for \mathbf{z}_0 an isolated zero of $f(\mathbf{x}) = 0$. Choose $\mathbf{h} \in \mathbb{C}^{\mathbb{R}+1}$ and $B \in \mathbb{C}^{n \times (\mathbb{R}+1)}$ at random.

Introduce $\mathbf{R} + 1$ new multiplier variables $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_{\mathbf{R}+1}).$

$$Dfl(f)(\mathbf{x}, \boldsymbol{\lambda}) := \begin{cases} f(\mathbf{x}) = \mathbf{0} & \operatorname{Rank}(J_f(\mathbf{x})) = \mathbf{R} \\ J_f(\mathbf{x})B\boldsymbol{\lambda} = \mathbf{0} & & \Downarrow \\ \mathbf{h}\boldsymbol{\lambda} = 1 & \operatorname{corank}(J_f(\mathbf{x})B) = 1 \end{cases}$$

Theorem (Anton Leykin, JV, Ailing Zhao):

The number of deflations needed to restore the quadratic convergence of Newton's method converging to an isolated solution is strictly less than the multiplicity.

deflation algorithm

Newton's Method with Deflation



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cyclic 9-roots revisited

Recall:

$$f(\mathbf{x}) = \begin{cases} f_i = \sum_{j=0}^8 \prod_{k=1}^i x_{(k+j) \mod 9} = 0, & i = 1, 2, \dots, 8\\ f_9 = x_0 x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 - 1 = 0 \end{cases}$$

has 164 solutions of multiplicity 4.

One deflation suffices to restore quadratic convergence.

The condition number drops from 1.8E+9 to 5.6E+2.

 \rightarrow deflation $\underline{reconditions}$ the system

Two Staircases with Different Local Ordering

Example: $I = \langle x_1^3 + x_1 x_2^2, x_1 x_2^2 + x_2^3, x_1^2 x_2 + x_1 x_2^2 \rangle$ in the ring $\mathbb{Q}[x_1, x_2], \mathbf{x}^* = \mathbf{0}, \boldsymbol{\omega}$ defines the monomial order.



: monomials generating $\mathbf{in}_{\omega}(I)$: standard monomials

#standard monomials = multiplicity of $x^* = 7$

Standard Bases and Dual Space

Consider

$$x_1^2 + 2x_2^2 - 2x_2 = 0$$
$$x_1x_2^2 - x_1x_2 = 0$$
$$x_2^3 - 2x_2^2 + x_2 = 0$$

from Möller-Stetter (1995).

$$\mathbf{z}_0 = (0, 0)$$

$$\mathbf{m}_0 = \mathbf{2}$$

$$D_0 = \operatorname{span}\{\partial_{00}, \partial_{10}\}$$

$$\mathbf{x}_2$$

$$\mathbf{x}_2$$

$$\mathbf{x}_1$$

 $\mathbf{z}_{1} = (0, 1) \text{ (shift to } (0, 0))$ $m_{1} = \mathbf{3}$ $D_{1} = \operatorname{span}\{\partial_{00}, \partial_{10}, 2\partial_{20} - \partial_{01}\}$



 $D[I] = D_0 \cup D_1$

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Effect of Deflation on the Staircase

 $I = \langle f_1 = x_1^3 + x_1 x_2^2, f_2 = x_1 x_2^2 + x_2^3, f_3 = x_1^2 x_2 + x_1 x_2^2 \rangle, \ \boldsymbol{\lambda} = (1, 1).$ $J = \langle f_1, f_2, f_3, \frac{\partial f_1}{\partial x_1} + \frac{\partial f_1}{\partial x_2}, \frac{\partial f_2}{\partial x_1} + \frac{\partial f_2}{\partial x_2}, \frac{\partial f_3}{\partial x_1} + \frac{\partial f_3}{\partial x_2} \rangle \text{ is a deflation of } I.$



: monomials generating $\mathbf{in}_{\omega}(I) \bigcirc$: standard monomials

m = 7 \longrightarrow m = 3 deflation

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One Deflation Step with fixed λ

- Assume corank(A(x*)) = 1.
 (reduce to this case with random combinations of columns)
- Let $\boldsymbol{\lambda} \in \ker(A(\mathbf{x}^*)), \, \boldsymbol{\lambda} \neq \mathbf{0}$, then for $g_i(\mathbf{x}) = \boldsymbol{\lambda} \cdot \nabla f_i = \sum_{j=1}^n \lambda_j \frac{\partial f_i}{\partial x_j}(x)$, we have: $g_i(\mathbf{x}^*) = \mathbf{0}$.

Theorem:

The augmented system
$$\left\{ egin{array}{ll} f_1 = f_2 = \cdots = f_N = 0 \ g_1 = g_2 = \cdots = g_N = 0 \
m{has x}^* \
m{as isolated root of lower multiplicity.} \end{array}
ight.$$

Proposition: Suppose m > 1 and let $g \in \mathcal{B}$, a reduced standard basis of I with respect to a local monomial ordering \leq , such that $g = x_i^d +$ lower order terms, for $i \in \{1, 2, ..., n\}$ and d > 1. Then $I' = I + \langle \frac{\partial g}{\partial x_i} \rangle$ is a **deflation** of I.

Lemma: Take a nonzero vector $\lambda \in \ker A(\mathbf{0}) \subset \mathbb{C}^n$ and let $\mathbf{x} = T(\mathbf{y})$ be a linear coordinate transformation such that

$$y_i = \lambda_i x_1 + \sum_{j=2}^n \mu_{ij} x_j, \quad \text{for } i = 1, 2, \dots, n,$$

where $\mathbf{y} = (y_1, \dots, y_n)$ are the new variables and $[\boldsymbol{\lambda}, \boldsymbol{\mu}_2, \dots, \boldsymbol{\mu}_n]$ is a nonsingular matrix. Let $T(I) = \{f(T(\mathbf{y})) \mid f \in I\} = \langle f_1(T(\mathbf{y})), \dots, f_N(T(\mathbf{y})) \rangle$ be the ideal after the change of coordinates. Then $\partial_1 T(I) = \left\{ \frac{\partial f}{\partial y_1} \mid f \in T(I) \right\}$ leads to a **deflation** of T(I).

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One Deflation Step with indeterminate λ

• Still assuming $\operatorname{corank}(A(\mathbf{x}^*)) = 1$.

• Denote
$$G(\mathbf{x}, \boldsymbol{\lambda}) = \begin{cases} g_i(\mathbf{x}, \boldsymbol{\lambda}) = \boldsymbol{\lambda} \cdot \nabla f_i(\mathbf{x}) = \mathbf{0} \\ \langle \mathbf{h}, \boldsymbol{\lambda} \rangle = h_1 \lambda_1 + h_2 \lambda_2 + \dots + h_n \lambda_n = 1. \end{cases}$$

Theorem:

Let $\mathbf{x}^* \in \mathbb{C}^n$ be an isolated singular root of $f(\mathbf{x}) = \mathbf{0}$ with multiplicity m. There exists a unique λ^* such that $\begin{cases} f(\mathbf{x}) = \mathbf{0} \\ G(\mathbf{x}, \lambda) = \mathbf{0} \end{cases}$ has $(\mathbf{x}^*, \lambda^*)$ as isolated root of multiplicity strictly less than m.

Proof: Consider $G(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{0}$ in the local ring $R_* = \mathbb{C}[\mathbf{x}, \boldsymbol{\lambda}]_{(\mathbf{x}^*, \boldsymbol{\lambda}^*)}$. Because $G(\mathbf{x}, \boldsymbol{\lambda})$ is linear in $\boldsymbol{\lambda}$, specializing $\mathbf{x} = \mathbf{x}^*$ turns $G(\mathbf{x}, \boldsymbol{\lambda}) = \mathbf{0}$ into a linear system with unique solution $\boldsymbol{\lambda}^*$.

> Using row operations in R_* , reduce $G(\mathbf{x}, \boldsymbol{\lambda})$ to the form :

$$\begin{cases} \lambda_1 = a_1(\mathbf{x}) \\ \vdots \\ \lambda_n = a_n(\mathbf{x}) \end{cases}$$

where $a_i(\mathbf{x})$ are rational expressions $(a_i(\mathbf{x}^*) = \lambda_i^*)$.

 $\begin{array}{ll} \text{multiplicity} & \left\{ \begin{array}{l} f(\mathbf{x}) = 0 \\ \text{of } \mathbf{x}^* \text{ in} \end{array} \right. \left\{ \begin{array}{l} f(\mathbf{x}) = 0 \\ G(\mathbf{x}, \boldsymbol{\lambda}) = 0 \end{array} \right. \Leftrightarrow & \text{multiplicity} \\ \text{of } \mathbf{x}^* \text{ in} \end{array} \left\{ \begin{array}{l} f(\mathbf{x}) = 0 \\ G(\mathbf{x}, \boldsymbol{\lambda}^*) = 0 \end{array} \right. \\ \text{local ring } \mathbb{C}[\mathbf{x}, \boldsymbol{\lambda}]_{(\mathbf{x}^*, \boldsymbol{\lambda}^*)} & \text{local ring } \mathbb{C}[\mathbf{x}]_{(\mathbf{x}^*)} \end{array} \right. \end{array}$

Computing the Multiplicity Structure

following B.H. Dayton and Z. Zeng

Looking for differentiation functionals
$$d[\mathbf{z}_0] = \sum_{\mathbf{a}} c_{\mathbf{a}} \partial_{\mathbf{a}}[\mathbf{z}_0],$$

with
$$\partial_{\mathbf{a}}[\mathbf{z}_0](p) = \frac{1}{a_1!a_2!\cdots a_n!} \left(\frac{\partial^{a_1+a_2+\cdots+a_n}}{\partial x_1^{a_1}\partial x_2^{a_2}\cdots \partial x_n^{a_n}} p \right) (\mathbf{z}_0).$$

Membership criterium for $d[\mathbf{z}_0]$:

 $d[\mathbf{z_0}] \in D_0 \Leftrightarrow d[\mathbf{z_0}](pf_i) = 0, \forall p \in \mathbb{C}[\mathrm{x}], i = 1, 2, \dots, N.$

To turning this criterium into an **algorithm**, observe:

- 1. since $d[\mathbf{z}_0]$ is linear, restrict p to $\mathbf{x}^{\mathbf{k}} = x_1^{k_1} x_2^{k_2} \cdots x_n^{k_n}$; and
- 2. limit degrees $k_1 + k_2 + \cdots + k_n \leq a_1 + a_2 + \cdots + a_n$, as $\mathbf{z}_0 = \mathbf{0}$ vanishes trivially if not annihilated by $\partial_{\mathbf{a}}$.

Computing the Multiplicity Structure – An Example

$$f_1 = x_1 - x_2 + x_1^2, f_2 = x_1 - x_2 + x_2^2$$

following B.H. Dayton and Z. Zeng

		a = 0	$a = 0 \qquad a = 1$		a =2			a =3			
		∂_{00}	∂_{10}	∂_{01}	∂_{20}	∂_{11}	∂_{02}	∂_{30}	∂_{21}	∂_{12}	∂_{03}
	f_1	0	1	-1	1	0	0	0	0	0	0
S_1	f_2	0	1	-1	0	0	1	0	0	0	0
	x_1f_1	0	0	0	1	-1	0	1	0	0	0
	$x_1 f_2$	0	0	0	1	-1	0	0	0	1	0
	$x_2 f_1$	0	0	0	0	1	-1	0	1	0	0
S_2	$x_2 f_2$	0	0	0	0	1	-1	0	0	0	1
	$x_{1}^{2}f_{1}$	0	0	0	0	0	0	1	-1	0	0
	$x_1^2 f_2$	0	0	0	0	0	0	1	-1	0	0
	$x_1 x_2 f_1$	0	0	0	0	0	0	0	1	-1	0
	$x_1 x_2 f_2$	0	0	0	0	0	0	0	1	-1	0
	$x_2^2 f_1$	0	0	0	0	0	0	0	0	1	-1
S_3	$x_{2}^{2}f_{2}$	0	0	0	0	0	0	0	0	1	-1

 $\operatorname{Nullity}(S_2) = \operatorname{Nullity}(S_3) \Rightarrow \operatorname{stop} \operatorname{algorithm}$

 $D_0 = \operatorname{span} \{ \partial_{00}, \partial_{10} + \partial_{01}, -\partial_{10} + \partial_{20} + \partial_{11} + \partial_{02} \} \Rightarrow \operatorname{multiplicity} = 3$

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cyclic 9-roots once more

Recall:

$$f(\mathbf{x}) = \begin{cases} f_i = \sum_{j=0}^8 \prod_{k=1}^i x_{(k+j) \mod 9} = 0, & i = 1, 2, \dots, 8\\ f_9 = x_0 x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 - 1 = 0 \end{cases}$$

has 164 solutions of multiplicity 4.

Running the algorithm of Dayton and Zeng:

$$egin{aligned} H[1] &= 1, H[2] = 2, H[3] = 1, H[4] = 0, \ ext{with} \ H[i] &= ext{Nullity}(S_i) - ext{Nullity}(S_{i-1}), i > 0, \end{aligned}$$

so we compute the multiplicity as 4.

Avoiding Expression Swell

Evaluation of $A(\mathbf{x})B$: for efficiency we must first replace \mathbf{x} by values *before* the matrix multiplication.

Triangular block structure of Jacobian matrix: for example:



Multipliers occur linearly: compute derivatives only with respect to \mathbf{x} , not with respect to $\boldsymbol{\lambda}$.

software & results

A Directed Acyclic Graph of Derivative Operators



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software & results

Numerical Results (double float)

System	n	m	D	$\operatorname{corank}(A(\mathbf{x}))$	Inverse Condition#	#Digits
baker1	2	2	1	1 ightarrow 0	$1.7e\text{-}08 \rightarrow 3.8e\text{-}01$	$9 \rightarrow 24$
cbms1	3	11	1	$3 \rightarrow 0$	$4.2\text{e-}05 \rightarrow 5.0\text{e-}01$	$5 \rightarrow 20$
cbms2	3	8	1	$3 \rightarrow 0$	$1.2e-08 \rightarrow 5.0e-01$	$8 \rightarrow 18$
mth191	3	4	1	$2 \rightarrow 0$	$1.3e-08 \rightarrow 3.5e-02$	$7 \rightarrow 13$
decker1	2	3	2	$1 \rightarrow 1 \rightarrow 0$	$3.4\text{e-}10 \rightarrow 2.6\text{e-}02$	$6 \rightarrow 11$
decker2	2	4	3	$1 \rightarrow 1 \rightarrow 1 \rightarrow 0$	$4.5\text{e-}13 \rightarrow 6.9\text{e-}03$	$5 \rightarrow 16$
decker3	2	2	1	1 ightarrow 0	$4.6\mathrm{e}\text{-}08 \rightarrow 2.5\mathrm{e}\text{-}02$	$8 \rightarrow 17$
ojika1	2	3	2	$1 \rightarrow 1 \rightarrow 0$	$9.3e-12 \rightarrow 4.3e-02$	$5 \rightarrow 12$
ojika2	3	2	1	1 ightarrow 0	$3.3e\text{-}08 \rightarrow 7.4e\text{-}02$	$6 \rightarrow 14$
ojika3	3	2	1	1 ightarrow 0	$1.7e\text{-}08 \rightarrow 9.2e\text{-}03$	$7 \rightarrow 15$
		4	1	$2 \rightarrow 0$	$6.5\mathrm{e}\text{-}08 \rightarrow 8.0\mathrm{e}\text{-}02$	$6 \rightarrow 13$
ojika4	3	3	2	1 ightarrow 1 ightarrow 0	$1.9e\text{-}13 \rightarrow 2.4e\text{-}04$	$6 \rightarrow 11$
cyclic9	9	4	1	$2 \rightarrow 0$	$5.6e-10 \rightarrow 1.8e-03$	$5 \rightarrow 15$

What is Symbolic-Numeric Computing?

A puristic point of view:

- **Computer algebra** rewrites the problem, producing "easier" equations of the ideal, but "easier" \neq numerically better.
- **Numerical analysis** produces approximate numbers for a fixed system of equations, but **many problems are "ill-posed**".

The synergistic approach:

Symbolic-Numeric Computing rewrites an ill-conditioned numerical problem into a well-conditioned formulation.

works very well in Newton's method with deflation

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