Computing Singularities using Newton’s Method with Deflation

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Computing Singular Isolated Roots

(Outline of the Talk)

1. Problem: Newton’s method fails for singular roots. Our goal is to restore quadratic convergence.

2. Deflation Algorithm: add linear combinations of derivatives. We rely on only one tolerance to determine the rank.

3. 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.

5. Prepares the computation of the multiplicity structure.
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);
- Allgower-Schwetlick (1995); Pönisch-Schnabel-Schwetlick (1999);

**computer algebra:** standard bases (SINGULAR)

**numerical polynomial algebra:** multiplicity structure
- Möller-Stetter (1995); Mourrain (1997); Stetter-Thallinger (1998);
- Dayton-Zeng (2005); Bates-Peterson-Sommese (2005)

**deflation:** Ojika-Watanabe-Mitsui (1983); Lecerf (2003)
Twelve lines tangent to four spheres

Frank Sottile and Thorsten Theobald: Lines tangents to $2n - 2$ spheres in $\mathbb{R}^n$


Problem:

Given 4 spheres,
find all lines tangent
to all 4 given spheres.

Observe:

12 solutions in groups of 4.
Twelve lines tangent to four spheres

Frank Sottile and Thorsten Theobald: Lines tangents to $2n - 2$ spheres in $\mathbb{R}^n$


Problem:
Given 4 spheres,
find all lines tangent
to all 4 given spheres.

Observe:
3 lines of multiplicity 4.
An Input Polynomial System

\begin{align*}
x_0^2 + x_1^2 + x_2^2 - 1; \\
x_0x_3 + x_1x_4 + x_2x_5; \\
x_3^2 + x_4^2 + x_5^2 - 0.25; \\
x_3^2 + x_4^2 - 2x_2x_4 + x_2^2 + x_5^2 + 2x_1x_5 + x_1^2 - 0.25; \\
x_3^2 + 1.73205080756888x_2x_3 + 0.75x_2^2 + x_4^2 - x_2x_4 + 0.25x_2^2 + x_5^2 - 1.73205080756888x_0x_5 + x_1x_5 + 0.75x_0^2 - 0.86602540378444x_0x_1 + 0.25x_1^2 - 0.25; \\
x_3^2 - 1.63299316185545x_1x_3 + 0.57735026918963x_2x_3 + 0.66666666666667x_1^2 - 0.47140452079103x_1x_2 + 0.08333333333333x_2^2 + x_4^2 + 1.63299316185545x_0x_4 - x_2x_4 + 0.66666666666667x_0^2 - 0.81649658092773x_0x_2 + 0.25x_2^2 + x_5^2 - 0.57735026918963x_0x_5 + x_1x_5 + 0.08333333333333x_0^2 - 0.28867513459481x_0x_1 + 0.25x_1^2 - 0.25; \\
\end{align*}

Original formulation as polynomial system: **Cassiano Durand**.
Centers of the spheres at the vertices of a tetrahedron: **Thorsten Theobald**.
**Algebraic numbers** \(\sqrt{3}, \sqrt{6}, \text{etc.} \) approximated by double floats.
**The system has 6 isolated solutions, each of multiplicity 4.**
Two solutions in a *cluster*:  

(Real and imaginary parts)

**Solution 1:**

<table>
<thead>
<tr>
<th>x0</th>
<th>-7.07106803165780E-01</th>
<th>3.77452918725401E-08</th>
</tr>
</thead>
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<tr>
<td>x1</td>
<td>-4.08248430737360E-01</td>
<td>-1.83624917064964E-07</td>
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<td>x3</td>
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<tr>
<td>x4</td>
<td>4.33012701892221E-01</td>
<td>-9.11600174682333E-17</td>
</tr>
<tr>
<td>x5</td>
<td>9.56878363411174E-08</td>
<td>1.54062878745083E-07</td>
</tr>
</tbody>
</table>

**Solution 2:**

<table>
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<th>-7.07106794356709E-01</th>
<th>-1.29682370414209E-07</th>
</tr>
</thead>
<tbody>
<tr>
<td>x1</td>
<td>-4.08248217029256E-01</td>
<td>1.11010906008961E-07</td>
</tr>
<tr>
<td>x2</td>
<td>5.77350304985648E-01</td>
<td>-8.03312536501087E-08</td>
</tr>
<tr>
<td>x3</td>
<td>-2.50000000000001E-01</td>
<td>-1.74789416181029E-16</td>
</tr>
<tr>
<td>x4</td>
<td>4.33012701892220E-01</td>
<td>-1.00914936462574E-16</td>
</tr>
<tr>
<td>x5</td>
<td>-6.07788020445124E-08</td>
<td>-1.39412292964849E-07</td>
</tr>
</tbody>
</table>

This is the **input** to our deflation algorithm.
A Benchmark Example: cyclic 9-roots

The system

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

has $333 \times 18$ isolated regular zeros, $164$ isolated 4-fold zeros, and $6$ cubic 2-dimensional irreducible solution components\(^a\).

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 . . .

A Simple Example

\[ f(x, y) = \begin{cases} 
  x^2 = 0 \\
  xy = 0 \\
  y^2 = 0 
\end{cases} \]

\( (0, 0) \) is an isolated root of multiplicity 3

Randomization or Embedding:

\[ \begin{cases} 
  x^2 + \gamma_1 y^2 = 0 \\
  xy + \gamma_2 y^2 = 0 
\end{cases} \quad \text{or} \quad \begin{cases} 
  x^2 + \gamma_1 z = 0 \\
  xy + \gamma_2 z = 0 \\
  y^2 + \gamma_3 z = 0 
\end{cases} \]

where \( \gamma_1, \gamma_2, \gamma_3 \in \mathbb{C} \) are random numbers and \( z \) is a slack variable,

*raises the multiplicity from 3 to 4!*

Simple to algebraic geometry, but not to numerical homotopies...
**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 $\Sigma$ ($N > n$).

The **condition number** $\text{cond}(J_f(z)) = \frac{\sigma_1}{\sigma_n}$.

$\text{Rank}(J_f(z)) = R \iff \Sigma = \text{diag}(\sigma_1, \sigma_2, \ldots, \sigma_R, 0, \ldots, 0)$.

At a **multiple root** $z_0$: $\text{Rank}(J_f(z_0)) = R < n$.

Close to $z_0$, $z \approx z_0 : \sigma_{R+1} \approx 0$, or $|\sigma_{R+1}| < \epsilon$, $\epsilon$ is tolerance.

**Moore-Penrose inverse**: $J_f^+ = V \Sigma^+ U^T$, with $R = \text{Rank}(J_f)$,
and $\Sigma^+ = \text{diag}(\frac{1}{\sigma_1}, \frac{1}{\sigma_2}, \ldots, \frac{1}{\sigma_R}, 0, \ldots, 0)$.

Then $\Delta z = -J_f(z)^+ f(z)$ is the least squares solution.

Dedieu-Shub (1999); Li-Zeng (2005)
The Simple Example – with deflation

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

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

\[ F(x, y, \lambda_1) = \begin{cases} 
  f(x, y) = 0 \\
  \begin{bmatrix} 2x & 0 \\ y & x \\ 0 & 2y \end{bmatrix} \begin{bmatrix} b_{11} \\ b_{21} \end{bmatrix} \lambda_1 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad \text{random} \ b_{11}, b_{21} \\
  h_1 \lambda_1 = 1, \quad \text{random} \ h_1 \in \mathbb{C} \end{cases} \]

The system \( F(x, y, \lambda_1) = 0 \) has \((0, 0, \lambda_1^*)\) as regular zero!
**Deflation Operator Dfl reduces to Corank One**

Consider $f(x) = 0$, $N$ equations in $n$ unknowns, $N \geq n$.

Suppose Rank($A(z_0)$) = $R < n$ for $z_0$ an isolated zero of $f(x) = 0$.

Choose $h \in \mathbb{C}^{R+1}$ and $B \in \mathbb{C}^{n \times (R+1)}$ at random.

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

\[
\text{Dfl}(f)(x, \lambda) := \begin{cases} 
   f(x) = 0 & \text{Rank}(A(x)) = R \\
   A(x)B\lambda = 0 & \downarrow \\
   h\lambda = 1 & \text{corank}(A(x)B) = 1
\end{cases}
\]

Compared to the deflation of Ojika, Watanabe, and Mitsui:
(1) we do not compute a maximal minor of the Jacobian matrix;
(2) we only add new equations, we never replace equations.
Newton’s Method with Deflation

**Input:** $f(x) = 0$ polynomial system;
- $x_0$ initial approximation for $x^*$;
- $\epsilon$ tolerance for numerical rank.
Newton’s Method with Deflation

**Input:** $f(x) = 0$ polynomial system; $x_0$ initial approximation for $x^*$; $\epsilon$ tolerance for numerical rank.

$[A^+, R] := \text{SVD}(A(x_k), \epsilon)$;

$x_{k+1} := x_k - A^+ f(x_k)$;

Gauss-Newton
Newton’s Method with Deflation

**Input:** $f(x) = 0$ polynomial system;
- $x_0$ initial approximation for $x^*$;
- $\epsilon$ tolerance for numerical rank.

$$[A^+, R] := \text{SVD}(A(x_k), \epsilon);$$
$$x_{k+1} := x_k - A^+ f(x_k);$$

**Gauss-Newton**

$$R = \#\text{columns}(A)?$$

**Yes**

**Output:** $f; x_{k+1}$.  

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deflation algorithm

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Newton’s Method with Deflation

**Input:** \( f(x) = 0 \) polynomial system; 
- \( x_0 \) initial approximation for \( x^* \); 
- \( \epsilon \) tolerance for numerical rank.

\[
\begin{align*}
[A^+, R] &= \text{SVD}(A(x_k), \epsilon); \\
x_{k+1} &= x_k - A^+ f(x_k);
\end{align*}
\]

\( R = \#\text{columns}(A) \)?

- Yes
  - **Output:** \( f; x_{k+1} \).

- No
  - **Deflation Step**
    \[
    \begin{align*}
    f &= \text{Dfl}(f)(x, \lambda) = \begin{cases} 
    f(x) = 0 \\
    G(x, \lambda) = 0
    \end{cases}; \\
    \hat{\lambda} &= \text{LeastSquares}(G(x_{k+1}, \lambda)); \\
    k &= k + 1; \\
    x_k &= (x_k, \hat{\lambda});
    \end{align*}
    \]
12 Lines Tangent to 4 Spheres revisited

Continuation methods find 24 solutions, clustered in groups of 4. The rank at all solutions is 4, corank is 2.

One deflation suffices to restore quadratic convergence.

An average condition number drops from $3.4E+8$ to $1.1E+2$.

We can compute the solutions with accuracy close to machine precision, on a system with approximate coefficients, given with double float precision.
Recall: \[ f(x) = \begin{cases} f_i = \sum_{j=0}^{8} \prod_{k=1}^{i} x_{(k+j) \mod 9} = 0, & i = 1, 2, \ldots, 8 \\ f_9 = x_0 x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 - 1 = 0 \end{cases} \]

has 164 solutions of multiplicity 4.

**One deflation suffices** to restore quadratic convergence.

An average **condition number** drops from 1.8E+9 to 5.6E+2.

\[ \rightarrow \text{deflation reconditions the problem} \]

A system with a cluster of solutions is close to a system with a multiple root.
<table>
<thead>
<tr>
<th>System</th>
<th>$n$</th>
<th>$m$</th>
<th>$D$</th>
<th>corank($A(x)$)</th>
<th>Inverse Condition#</th>
<th>#Digits</th>
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<td>3</td>
<td>1</td>
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<td>$1.0e-08 \rightarrow 4.1e-01$</td>
<td>8 $\rightarrow$ 24</td>
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<td>2</td>
<td>1</td>
<td>$1 \rightarrow 0$</td>
<td>$1.7e-08 \rightarrow 3.8e-01$</td>
<td>9 $\rightarrow$ 24</td>
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<td>cbms1</td>
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<td>$9 \rightarrow 0$</td>
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</table>
Some Remaining Questions ...

1) Does the deflation algorithm terminate?
2) Is the deflation algorithm efficient?
3) How to compute the multiplicity of a root?
Ideals, Quotient Rings, and Dual Spaces

- Ideal $I$
- Quotient ring $R[I]$
- Dual space $D[I]$

A commutative diagram
$P(x) = 0$

$P = (p_1, p_2, \ldots, p_N)$

$I = \{ \sum_{k=1}^{N} c_k(x)p_k \mid c_k \in \mathbb{C}[x] \}$

$Z[I] = \{ z \in \mathbb{C}^n \mid p(z) = 0, \forall p \in I \}$

$a \text{ commutative diagram}$
Ideals, Quotient Rings, and Dual Spaces

\[ P(x) = 0 \]
\[ P = (p_1, p_2, \ldots, p_N) \]
\[ p_k \in \mathbb{C}[x] \]

**ideal** \[ I = \langle P \rangle = \{ \sum_{k=1}^{N} c_k(x)p_k \mid c_k \in \mathbb{C}[x] \} \]

**Z[I]** \[ Z[I] = \{ z \in \mathbb{C}^n \mid p(z) = 0, \forall p \in I \} \]

**quotient ring** \[ R[I] = \{ [p]_I \mid p \in \mathbb{C}[x] \} \]
**residue class ring**, compute modulo \( I \)

\[ [p]_I = \{ r \in \mathbb{C}[x] \mid p - r \in I \} = \{ r \in \mathbb{C}[x] \mid p(z) = r(z), \forall z \in Z[I] \} \]

**dual space** \[ D[I] \]
Ideals, Quotient Rings, and Dual Spaces

\[ P(x) = 0 \]
\[ P = (p_1, p_2, \ldots, p_N) \]
\[ p_k \in \mathbb{C}[x] \]

**ideal** \( I = \langle P \rangle = \left\{ \sum_{k=1}^{N} c_k(x)p_k \mid c_k \in \mathbb{C}[x] \right\} \)

\[ Z[I] = \left\{ z \in \mathbb{C}^n \mid p(z) = 0, \forall p \in I \right\} \]

**quotient ring** \( R[I] = \{ [p]_I \mid p \in \mathbb{C}[x] \} \)
\[ [p]_I = \{ r \in \mathbb{C}[x] \mid p - r \in I \} \]

**dual space** \( D[I] = \{ l : \mathbb{C}[x] \to \mathbb{C}, l(p) = 0, \forall p \in I \} \)
Ideals, Quotient Rings, and Dual Spaces

\[ P(x) = 0 \]
\[ P = (p_1, p_2, \ldots, p_N) \]
\[ p_k \in \mathbb{C}[x] \]
\[ \text{ideal } I = \langle P \rangle = \{ \sum_{k=1}^{N} c_k(x)p_k \mid c_k \in \mathbb{C}[x] \} \]
\[ Z[I] = \{ \mathbf{z} \in \mathbb{C}^n \mid p(\mathbf{z}) = 0, \forall p \in I \} \]

**Theorem:** If \( \#Z[I] < \infty \), then \( \dim(R[I]) = \#Z[I] \).

\[ I \to R[I] \] interpolation at \( Z[I] \) gives basis for \( R[I] \).

\[ R[I] \to I \] for some basis \( \mathbf{b} \) of \( R[I] \),
\[ A_k \mathbf{b} = x_k \mathbf{b} \] yields border basis.
The dual space of the quotient ring $R[I]$:

$$(R[I])^* = \{ l : R[I] \to \mathbb{C} : [p]_I \mapsto l(p) := l(r), r \in R[I], p - r \in I \}.$$  

**Theorem:** $D[I] = (R[I])^*$ and $R[I] = (D[I])^*$.

Note: $I[D[I]] = \{ p \in \mathbb{C}[x] : l(p) = 0, \forall l \in D[I] \} = I$.

The dual includes “the multiplicity structure” of the solutions.

**Diagram:**

- $\mathbb{R}[I]$ \hspace{2cm} quotient ring
- $D[I]$ \hspace{2cm} dual space

$R[I] = \{ [p]_I \mid p \in \mathbb{C}[x] \}$

$[p]_I = \{ r \in \mathbb{C}[x] \mid p - r \in I \}$

$D[I] = \{ l : \mathbb{C}[x] \to \mathbb{C}, l(p) = 0, \forall p \in I \}$
Multiplicy of an Isolated Zero via Duality

Analogy with Univariate Case: \( z_0 \) is \( m \)-fold zero of \( f(x) = 0 \):
\[
\begin{align*}
  f(z_0) &= 0, \\
  \frac{\partial f}{\partial x}(z_0) &= 0, \\
  \frac{\partial^2 f}{\partial x^2}(z_0) &= 0, \\
  & \vdots \\
  \frac{\partial^{m-1} f}{\partial x^{m-1}}(z_0) &= 0 \\
\end{align*}
\]

\( m \) = number of linearly independent polynomials annihilating \( z_0 \).

The dual space \( D_0 \) at \( z_0 \) is spanned by \( m \) linear independent differentiation functionals annihilating \( z_0 \).

Consider again
\[
f(x, y) = \begin{cases} 
  x^2 = 0 \\
  xy = 0 \\
  y^2 = 0 
\end{cases}
\]

The multiplicity of \( z_0 = (0, 0) \) is \( 3 \) because

\[
D_0 = \text{span}\{\partial_{00}[z_0], \partial_{10}[z_0], \partial_{01}[z_0]\}, \text{ with } \partial_{ij}[z_0] = \frac{1}{i!j!} \frac{\partial^{i+j}}{\partial x^i \partial y^j} f(z_0).
\]
Standard Bases and Dual Space

Consider
\[
\begin{align*}
  x_1^2 + 2x_2^2 - 2x_2 &= 0 \\
  x_1x_2^2 - x_1x_2 &= 0 \\
  x_2^3 - 2x_2^2 + x_2 &= 0
\end{align*}
\]

\[z_0 = (0, 0)\]
\[m_0 = 2\]
\[D_0 = \text{span}\{\partial_{00}, \partial_{10}\}\]

\[z_1 = (0, 1) \text{ (shift to } (0,0)\text{)}\]
\[m_1 = 3\]
\[D_1 = \text{span}\{\partial_{00}, \partial_{10}, 2\partial_{20} - \partial_{01}\}\]

\[D[I] = D_0 \cup D_1\]
Two Staircases with Different Local Ordering

Example: \( I = \langle x_1^3 + x_1x_2^2, x_1x_2^2 + x_2^3, x_1^3x_2 + x_1x_2^2 \rangle \) in the ring \( \mathbb{Q}[x_1, x_2], \mathbf{x}^* = 0, \omega \) defines a local monomial order. 

\[
\begin{align*}
\omega &= (-1, -2) \\
\omega &= (-2, -1)
\end{align*}
\]

\( \bullet \): monomials generating \( \text{in}_\omega(I) \) 
\( \bigcirc \): standard monomials

\#standard monomials = multiplicity of \( \mathbf{x}^* = 7 \)
why it works

Effect of Deflation on the Staircase

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

\[ \omega = (-1, -2) \]

\( \bullet \): monomials generating \( \text{in}_\omega(I) \)

\( \bigcirc \): standard monomials

\[ m = 7 \quad \text{deflation} \quad m = 3 \]
One Deflation Step with fixed $\lambda$

- Assume $\text{corank}(A(x^*)) = 1$.
  
  (reduce to this case with random combinations of columns)

- Let $\lambda \in \ker(A(x^*)), \lambda \neq 0$,
  
  then for $g_i(x) = \lambda \cdot \nabla f_i = \sum_{j=1}^{n} \lambda_j \frac{\partial f_i}{\partial x_j}(x)$, we have: $g_i(x^*) = 0$.

**Theorem:**

The augmented system

\[
\begin{cases}
    f_1 = f_2 = \cdots = f_N = 0 \\
    g_1 = g_2 = \cdots = g_N = 0
\end{cases}
\]

has $x^*$ as isolated root of lower multiplicity.
**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 $g = x_i^d + \text{lower order terms}$, for $i \in \{1, 2, \ldots, n\}$ and $d > 1$. Then $I' = I + \langle \frac{\partial g}{\partial x_i} \rangle$ is a deflation of $I$.

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

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

where $y = (y_1, \ldots, y_n)$ are the new variables and $[\lambda, \mu_2, \ldots, \mu_n]$ is a nonsingular matrix.

Let $T(I) = \{ f(T(y)) \mid f \in I \} = \langle f_1(T(y)), \ldots, f_N(T(y)) \rangle$ 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 $T(I)$.
One Deflation Step with indeterminate $\lambda$

- Still assuming $\text{corank}(A(x^*)) = 1$.

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

**Theorem:**

Let $x^* \in \mathbb{C}^n$ be an isolated singular root of $f(x) = 0$ with multiplicity $m$. There exists a unique $\lambda^*$ such that $\begin{cases} f(x) = 0 \\
G(x, \lambda) = 0 \end{cases}$ has $(x^*, \lambda^*)$ as isolated root of multiplicity strictly less than $m$. 
Proof: Consider $G(x, \lambda) = 0$ in the local ring $R_\star = \mathbb{C}[x, \lambda]_{(x^\star, \lambda^\star)}$. Because $G(x, \lambda)$ is linear in $\lambda$, specializing $x = x^\star$ turns $G(x, \lambda) = 0$ into a linear system with unique solution $\lambda^\star$.

Using row operations in $R_\star$, reduce $G(x, \lambda)$ to the form:

$$
\begin{align*}
\lambda_1 &= a_1(x) \\
\vdots \\
\lambda_n &= a_n(x)
\end{align*}
$$

where $a_i(x)$ are rational expressions ($a_i(x^\star) = \lambda_i^\star$).

Multiplicity of $x^\star$ in $\mathbb{C}[x, \lambda]_{(x^\star, \lambda^\star)}$ is equivalent to multiplicity of $x^\star$ in $\mathbb{C}[x]_{(x^\star)}$ for $f(x) = 0$.

$$
\begin{align*}
\text{Multiplicity of } x^\star \text{ in } & \mathbb{C}[x, \lambda]_{(x^\star, \lambda^\star)} \\
\implies \text{Multiplicity of } x^\star \text{ in } & \mathbb{C}[x]_{(x^\star)}
\end{align*}
$$
**A Bound on the Number of Deflations**

**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.

Duality Analysis of Barry H. Dayton and Zhonggang Zeng:

(1) tighter bound on number of deflations; and

(2) special case algorithms, for corank = 1.

(Proceedings of ISSAC 2005)
Avoiding Expression Swell

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

Triangular block structure of Jacobian matrix: for example:

$$A_2(x, \lambda_1, \lambda_2) = \begin{bmatrix}
  A & 0 & 0 \\
  (\frac{\partial A}{\partial x}) B_1 \lambda_1 & AB_1 & 0 \\
  0 & h_1 & 0 \\
  (\frac{\partial A_1}{\partial x}) B_2 \lambda_2 & \left(\frac{\partial A_1}{\partial \lambda_1}\right) B_2 \lambda_2 & A_1 B_2 \\
  0 & 0 & h_2
\end{bmatrix}.$$  

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

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**Structure of the Deflated Systems**

At stage $k$ in the deflation:

$$f_k(x, \lambda_1, \ldots, \lambda_{k-1}, \lambda_k) = \begin{cases} f_{k-1}(x, \lambda_1, \ldots, \lambda_{k-1}) = 0 \\ A_{k-1}(x, \lambda_1, \ldots, \lambda_{k-1})B_k \lambda_k = 0 \\ h_k \lambda_k = 1, \end{cases}$$

$f_0 = f$, $A_0 = A$, $R_k = \text{rank}(A_{k-1}(z_0))$, $R_k + 1$ multipliers in $\lambda_k$. random vector $h_k \in \mathbb{C}^{R_k+1}$ and $n_{k-1}$-by-$(R_k + 1)$ matrix $B_k$

$$\#\text{rows in } A_k : N_k = 2N_{k-1} + 1, \quad N_0 = N,$$

$$\#\text{columns in } A_k : n_k = n_{k-1} + R_k + 1, \quad n_0 = n.$$

Multiplication of the polynomial matrix $A_{k-1}$ with the random matrix $B_k$ and vector of $R_k + 1$ multiplier variables $\lambda_k$ is expensive!
Structure of the Jacobian Matrices

At stage $k$ in the deflation:

\[
f_k(x, \lambda_1, \ldots, \lambda_{k-1}, \lambda_k) = \begin{cases} 
  f_{k-1}(x, \lambda_1, \ldots, \lambda_{k-1}) = 0 \\
  A_{k-1}(x, \lambda_1, \ldots, \lambda_{k-1}) B_k \lambda_k = 0 \\
  h_k \lambda_k = 1 
\end{cases}
\]

Jacobian matrix at the $k$th deflation:

\[
A_k(x, \lambda_1, \ldots, \lambda_{k-1}, \lambda_k) = \begin{bmatrix} 
  A_{k-1} & 0 \\
  \frac{\partial A_{k-1}}{\partial x} & \frac{\partial A_{k-1}}{\partial \lambda_1} & \ldots & \frac{\partial A_{k-1}}{\partial \lambda_{k-1}} \\
  0 & B_k \lambda_k & A_{k-1} B_k \\
  h_k & & & h_k 
\end{bmatrix}
\]

The multiplier variables $\lambda_i$, $i = 1, 2, \ldots, k$, occur linearly, we compute derivatives only with respect to the original variables $x$. 
Derivatives of Jacobian matrices

Define \( \frac{\partial A}{\partial x} = \left[ \frac{\partial A}{\partial x_1} \frac{\partial A}{\partial x_2} \cdots \frac{\partial A}{\partial x_n} \right] \), \( x = (x_1, x_2, \ldots, x_n) \),

where \( \frac{\partial A}{\partial x_k} = \left[ \frac{\partial a_{ij}}{\partial x_k} \right] \) for \( A = [a_{ij}(x)]_{i,j \in \{1,2,\ldots,N\}} \).

Natural tree structure:
(to compute \( \frac{\partial^2 A}{\partial x^2} \))

\[
A(x_1, x_2) \\
\frac{\partial A}{\partial x_1} \quad \frac{\partial A}{\partial x_2} \\
\frac{\partial^2 A}{\partial x^2} \quad \frac{\partial^2 A}{\partial x_1 \partial x_2} = \frac{\partial^2 A}{\partial x_1 \partial x_2} \quad \frac{\partial^2 A}{\partial x_2^2}
\]

Complexity of \( \frac{\partial^k A}{\partial x^k} \neq O(n^k) \),
but \( O(\#\text{monomials of degree } k \text{ in } n \text{ variables}) \).

\( k = 10, n = 3: \quad 3^{10} = 59049 \gg 66 \)
Column Format of Jacobian Matrices

Jacobian matrix at the $k$th deflation:

$$A_k(x, \lambda_1, \ldots, \lambda_{k-1}, \lambda_k) = \begin{bmatrix} A_{k-1} \\ \frac{\partial A_{k-1}}{\partial x} & \frac{\partial A_{k-1}}{\partial \lambda_1} & \cdots & \frac{\partial A_{k-1}}{\partial \lambda_{k-1}} \\ 0 \\ B_k \lambda_k & A_{k-1} B_k \\ h_k \end{bmatrix}.$$ 

Tree with $k$ children:

$$A_k(x, \lambda_1, \ldots, \lambda_{k-1}, \lambda_k)$$

$$\xrightarrow{A_{k-1}} \xrightarrow{\frac{\partial A_{k-1}}{\partial x}} \xrightarrow{\frac{\partial A_{k-1}}{\partial \lambda_1}} \cdots \xrightarrow{\frac{\partial A_{k-1}}{\partial \lambda_{k-1}}}$$
Unwinding the Multipliers

\[
A_2(x, \lambda_1, \lambda_2) = \begin{bmatrix}
A_1 & 0 \\
\frac{\partial A_1}{\partial x} & \frac{\partial A_1}{\partial \lambda_1} & B_2\lambda_2 & A_1B_2 \\
0 & h_2
\end{bmatrix}
\]
Unwinding the Multipliers

\[ A_2(x, \lambda_1, \lambda_2) = \begin{bmatrix} A_1 & 0 \\ \frac{\partial A_1}{\partial x} & \frac{\partial A_1}{\partial \lambda_1} \end{bmatrix} B_2 \lambda_2 \begin{bmatrix} A_1 B_2 \\ h_2 \end{bmatrix} \]

Directed Acyclic Graph:
The Operator *

For a matrix $B$: 
\[
\left[ \frac{\partial A}{\partial x} \right] B = \left[ \frac{\partial A}{\partial x_1} B \; \frac{\partial A}{\partial x_2} B \; \cdots \; \frac{\partial A}{\partial x_n} B \right].
\]

However, 
\[
\frac{\partial}{\partial \lambda} \left( \left[ \frac{\partial A}{\partial x} \right] B \lambda \right) = 
\begin{bmatrix}
\frac{\partial A}{\partial x} b_1 & \frac{\partial A}{\partial x} b_2 & \cdots & \frac{\partial A}{\partial x} b_m \\
\partial \lambda_1 & \partial \lambda_2 & \cdots & \partial \lambda_m
\end{bmatrix},
\]

where 
\[
\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_m), \quad B = [b_1 \; b_2 \; \cdots \; b_m].
\]

Unlike scalar differentiation: 
\[
\frac{\partial}{\partial \lambda} \left( \left[ \frac{\partial A}{\partial x} \right] B \lambda \right) \neq \left[ \frac{\partial A}{\partial x} \right] B.
\]

With the operator * we permute $\left[ \frac{\partial A}{\partial x} \right] B$ into 
\[
\frac{\partial}{\partial \lambda} \left( \left[ \frac{\partial A}{\partial x} \right] B \lambda \right).
\]

So we have: 
\[
\frac{\partial}{\partial \lambda} \left( \left[ \frac{\partial A}{\partial x} \right] B \lambda \right) = \left[ \frac{\partial A}{\partial x} \right] * B.
\]
A Directed Acyclic Graph of Derivative Operators

\[ A_3(x, \lambda_1, \lambda_2, \lambda_3) \]

\[ A_2(x, \lambda_1, \lambda_2) \]
\[ \frac{\partial A_2}{\partial x} \quad \frac{\partial A_2}{\partial \lambda_1} \quad \frac{\partial A_2}{\partial \lambda_2} \]

\[ A_1(x, \lambda_1) \]
\[ \frac{\partial A_1}{\partial x} \quad \frac{\partial A_1}{\partial \lambda_1} \quad \frac{\partial^2 A_1}{\partial x^2} \quad \frac{\partial^2 A_1}{\partial x \partial \lambda_1} \]

\[ A(x) \]
\[ \frac{\partial A}{\partial x} \quad \frac{\partial^2 A}{\partial x^2} \quad \frac{\partial^3 A}{\partial x^3} \]
The growth of the number of nodes in the directed acyclic graph, for increasing deflations $k$:

<table>
<thead>
<tr>
<th>$k$</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
<th>8</th>
<th>9</th>
<th>10</th>
</tr>
</thead>
<tbody>
<tr>
<td>#nodes</td>
<td>3</td>
<td>7</td>
<td>14</td>
<td>26</td>
<td>46</td>
<td>79</td>
<td>133</td>
<td>221</td>
<td>364</td>
<td>596</td>
</tr>
</tbody>
</table>

#nodes ranges between $O(k^2)$ and $O(k^3)$
Computing the Multiplicity Structure

following B.H. Dayton and Z. Zeng, ISSAC 2005

Looking for differentiation functionals \( d[z_0] = \sum_a c_a \partial_a[z_0] \),

with \( \partial_a[z_0](p) = \frac{1}{a_1!a_2!\cdots a_n!} \left( \frac{\partial^{a_1+a_2+\cdots+a_n}}{\partial x_1^{a_1}\partial x_2^{a_2}\cdots\partial x_n^{a_n}} p \right)(z_0) \).

Membership criterium for \( d[z_0] \):

\[
d[z_0] \in D_0 \iff d[z_0](pf_i) = 0, \forall p \in \mathbb{C}[x], i = 1, 2, \ldots, N.
\]

To turning this criterium into an algorithm, observe:

1. since \( d[z_0] \) is linear, restrict \( p \) to \( x^k = x_1^{k_1}x_2^{k_2}\cdots x_n^{k_n} \); and

2. limit degrees \( k_1 + k_2 + \cdots + k_n \leq a_1 + a_2 + \cdots + a_n \),
as \( z_0 = 0 \) vanishes trivially if not annihilated by \( \partial_a \).
Computing the Multiplicity Structure – An Example

\( f_1 = x_1 - x_2 + x_1^2, \quad f_2 = x_1 - x_2 + x_2^2 \)  following B.H. Dayton and Z. Zeng

|   | \( |a| = 0 \) | \( |a| = 1 \) | \( |a| = 2 \) | \( |a| = 3 \) |
|---|---|---|---|---|
|   | \( \partial_{00} \) | \( \partial_{10} \) | \( \partial_{01} \) | \( \partial_{20} \) | \( \partial_{11} \) | \( \partial_{02} \) | \( \partial_{30} \) | \( \partial_{21} \) | \( \partial_{12} \) | \( \partial_{03} \) |
| \( S_1 \) | \( f_1 \) | 0 | 1 | -1 | 1 | 0 | 0 | 0 | 0 | 0 |
| \( f_2 \) | 0 | 1 | -1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 |
| \( x_1 f_1 \) | 0 | 0 | 0 | 1 | -1 | 0 | 0 | 0 | 0 | 0 |
| \( x_1 f_2 \) | 0 | 0 | 0 | 1 | -1 | 0 | 0 | 0 | 0 | 0 |
| \( x_2 f_1 \) | 0 | 0 | 0 | 0 | 1 | -1 | 0 | 0 | 0 | 0 |
| \( x_2 f_2 \) | 0 | 0 | 0 | 0 | 1 | -1 | 0 | 0 | 0 | 0 |
| \( S_2 \) | \( x_1^2 f_1 \) | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -1 | 0 |
| \( x_1^2 f_2 \) | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -1 | 0 |
| \( x_1 x_2 f_1 \) | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -1 | 0 |
| \( x_1 x_2 f_2 \) | 0 | 0 | 0 | 0 | 0 | 0 | 1 | -1 | 0 |
| \( x_2^2 f_1 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |
| \( x_2^2 f_2 \) | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 |

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

\( D_0 = \text{span}\{ \partial_{00}, \partial_{10} + \partial_{01}, -\partial_{10} + \partial_{20} + \partial_{11} + \partial_{02} \} \Rightarrow \text{multiplicity} = 3 \)
cyclic 9-roots once more

Recall:

\[
f(x) = \begin{cases} 
  f_i = \sum_{j=0}^{8} \prod_{k=1}^{i} x^{(k+j) \mod 9} = 0, & i = 1, 2, \ldots, 8 \\
  f_9 = x_0x_1x_2x_3x_4x_5x_6x_7x_8 - 1 = 0
\end{cases}
\]

has 164 solutions of multiplicity 4.

Running the algorithm of Dayton and Zeng:

\[
\]

with \( H[i] = \text{Nullity}(S_i) - \text{Nullity}(S_{i-1}) \), \( i > 0 \),

so we compute locally the multiplicity as 4.
12 Lines Tangent to 4 Spheres once more

With deflation 6 solutions of multiplicity 4 are computed accurately, i.e.: the cluster radius is close to machine precision.

Running the algorithm of Dayton and Zeng:


with \[ H[i] = \text{Nullity}(S_i) - \text{Nullity}(S_{i-1}), i > 0, \]

so we compute locally the multiplicity as 4.
Concluding Remarks

software at http://www.math.uic.edu/~jan/download.html

papers with Anton Leykin and Ailing Zhao

- Newton’s Method with Deflation for Isolated Singularities of Polynomial Systems.
  To appear in *Theoretical Computer Science*.
