Newton's Method with Deflation for Isolated Singularities

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0. Setup and Motivation

Let $F(\mathbf{x}) = \mathbf{0}$ be a polynomial system, with $\mathbf{x} \in \mathbb{C}^n$.
We are interested in $\mathbf{x}^*$, an *isolated* solution of $F(\mathbf{x}) = \mathbf{0}$:

$$\text{for small enough } \epsilon > 0 : \{ \mathbf{y} \in \mathbb{C}^n : ||\mathbf{y} - \mathbf{x}^*|| < \epsilon \} \cap F^{-1}(\mathbf{0}) = \{\mathbf{x}^*\}.$$

Denote by $A(\mathbf{x})$ the Jacobi matrix of the system $F(\mathbf{x}) = \mathbf{0}$.
We call $\mathbf{x}^*$ a *singular* solution of $F(\mathbf{x}) = \mathbf{0} \Leftrightarrow \mathrm{Rank}(A(\mathbf{x}^*)) < n$.
Let m be the *multiplicity* of the isolated solution $\mathbf{x}^*$ of $F(\mathbf{x}) = \mathbf{0}$.

Newton's method generates a sequence of approximations $\mathbf{x}_k$ for $\mathbf{x}^*$
+ $\|\mathbf{x}_k - \mathbf{x}_{k+1}\| = O(\|\mathbf{x}_{k-1} - \mathbf{x}_k\|^2)$, for $\mathbf{x}^*$ nonsingular; but
− convergence slows down or is lost when $\mathbf{x}_k \approx \mathbf{x}^*$ for $\mathbf{x}^*$ singular.

Brutal force: using $m \times D$ decimal places in working precision to achieve D correct decimal places in final approximation only works if coefficients in system F have their first $m \times D$ decimal places correct!

Goal: restore quadratic convergence without extra requirements of precision on F.

1. A Modified Deflation Method

A singular root $\mathbf{x}^*$ of a square system $F(\mathbf{x}) = \mathbf{0}$ satisfies $\begin{cases} F(\mathbf{x}) = \mathbf{0} \\ \det(A(\mathbf{x})) = 0, \end{cases}$

which forms the basis of deflation, as adapted and modified in [1], [2], and [3].

In theory, $\det(A(\mathbf{x})) = 0$ (or maximal minors) could be used as new equations.
But: 1. high in degree: expression swell; and moreover
2. numerically unstable: $\| \det(A(\mathbf{x})) - \det(\overline{A}(\mathbf{x}))\| \gg \|A(\mathbf{x}) - \overline{A}(\mathbf{x})\|$.

Three steps to set up new equations:

1. Obtain $R = \mathrm{Rank}(A(\mathbf{x}))$ for $\mathbf{x} \approx \mathbf{x}^*$ using Singular Value Decomposition(SVD).
2. Generate a random vector $\alpha \in \mathbb{C}^{R+1}$ and a random matrix $\beta \in \mathbb{C}^{n \times (R+1)}$.
3. Let $C = A\beta, C = [\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_{R+1}]$, adding $R+1$ new unknowns.

$$\det(A(\mathbf{x}^*)) = 0 \Leftrightarrow \det([\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_n]) = 0$$

$$\Leftrightarrow \exists \lambda_1, \lambda_2, \ldots, \lambda_{R+1} : G(\mathbf{x}, \lambda) = \begin{cases} \displaystyle\sum_{i=1}^{R+1} \lambda_i \mathbf{c}_i = \mathbf{0} \\ \displaystyle\sum_{i=1}^{R+1} \alpha_i \lambda_i = 1 \end{cases}$$

where $\mathbf{a}_i = [a_{1i}, a_{2i}, \ldots, a_{ni}], \mathbf{c}_i = [c_{1i}, c_{2i}, \ldots, c_{ni}]$.
The random α and β guarantee there is a unique solution for λ.
Add $G(\mathbf{x}, \lambda)$ instead of $\det(A(\mathbf{x})) = 0$ to the system $F(\mathbf{x}) = \mathbf{0}$.

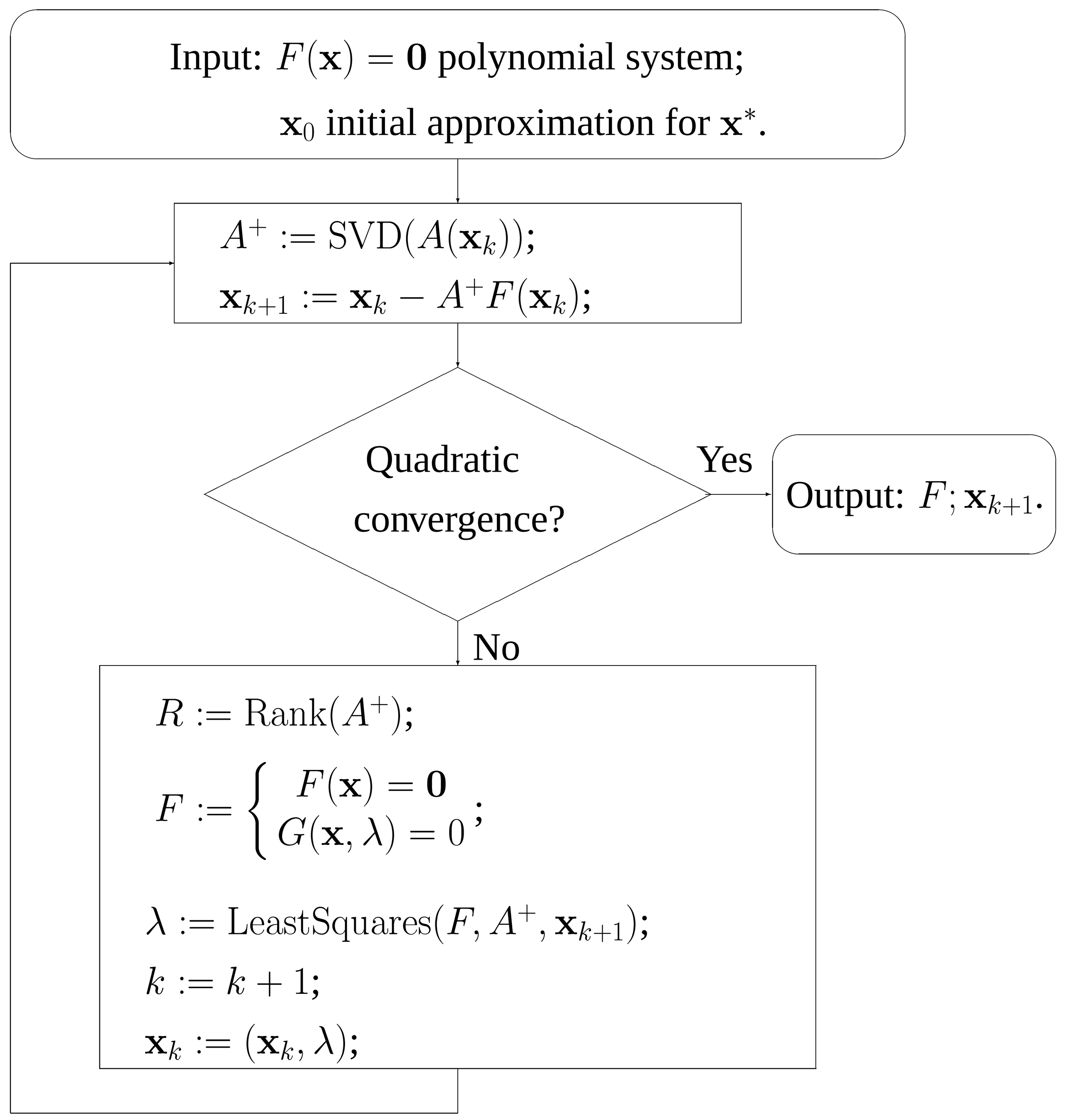
References

[1] T. Ojika, S. Watanabe, and T. Mitsui. **Deflation algorithm for the multiple roots of a system of nonlinear equations.** *J. Math. Anal. Appl.* 96, 463–479, 1983.

[2] T. Ojika. **Modified deflation algorithm for the solution of singular problems. I. A system of nonlinear algebraic equations.** *J. Math. Anal. Appl.* 123:199–221, 1987.

[3] T. Ojika. **Modified deflation algorithm for the solution of singular problems. II. Nonlinear multipoint boundary value problems.** *J. Math. Anal. Appl.* 123: 222–237, 1987.

2. Flowchart for Newton's Method with Deflation



3. A Bound on the Number of Deflations

Lemma 1 *If $\mathbf{x}^*$ is an isolated solution of the original system, then $(\mathbf{x}^*, \lambda^*)$ is also an isolated solution of the deflated system.*

Proof. $\mathrm{rank}(A) = R \Leftrightarrow$ any $R+1$ combinations of columns of A gives a zero determinant. The last added equation guarantees a unique value for λ^*.

Lemma 2 *Deflations do never increase the corank of the Jacobian matrix.*

Proof. The new Jacobian matrix $\widetilde{A}$ has the following block matrix structure.

$$\left(\begin{array}{c|c} A & 0 \\ \hline S & A\beta \\ \hline 0 & \alpha \end{array} \right)$$

where A is the original Jacobian matrix, S consists of random combinations of second derivatives of the original polynomials, and $A\beta$ is the result of the multiplication of A with a random matrix β.
Denote $R = \mathrm{rank}(A(\mathbf{x}^*)), \mathrm{corank}(A(\mathbf{x}^*)) = n - R$.
$\mathrm{rank}(\beta) = R + 1 \Rightarrow \mathrm{rank}(A\beta) = R$, thus
$\mathrm{rank}(\widetilde{A}) \geq 2R + 1 \Rightarrow \mathrm{corank}(\widetilde{A}) \leq n + R + 1 - (2R+1) \leq n - R$.

Conjecture 3 *The number of deflations needed to restore quadratic convergence of Newton's method to an isolated solution is strictly less than its multiplicity.*

Ojika, Watanabe, and Mitsui proved this bound on the number of deflations in the case of $f_i(\mathbf{x}) = (a_{i1}x_1 + \cdots + a_{i,i-1}x_{i-1} + x_i + a_{i,i+1}x_{i+1} + \cdots + a_{in}x_n)^{m_i} \widetilde{f}_i(\mathbf{x}) = 0$, where $f_i(\mathbf{x}^*) = 0, \widetilde{f}_i(\mathbf{x}^*) \neq 0, i = 1, 2, \ldots, n$.

4. A Symbolic-Numeric Implementation

The method was tested and developed in Maple 9. It is implemented in PHCpack [6], publicly available in release 2.3. While floating-point arithmetic is used, the result is symbolic, in the form of a new polynomial system with a well conditioned root.

5. Applications and Numerical Results

The implementation has been tested on seventeen examples, available at `http://www.math.uic.edu/~jan/demo.html`. The initial approximations for Newton's method were taken from the end points of solution paths defined by a homotopy. The numerical results reported in the table below are obtained with standard machine arithmetic. Observe the improved numerical conditioning.

System	m	#Deflations	Rank	Inverse Condition#
eg1	4	1	$0 \rightarrow 3$	8.3e-09→ 5.0e-01
eg2	2	1	$1 \rightarrow 4$	1.2e-08→ 1.8e-01
eg3	2	1	$1 \rightarrow 4$	5.6e-09→ 1.2e-01
eg4	3	2	$1 \rightarrow 3 \rightarrow 8$	3.0e-10→ 6.4e-02
eg5	4	3	$1 \rightarrow 3 \rightarrow 7 \rightarrow 16$	6.4e-11→ 5.7e-03
baker1	2	1	$1 \rightarrow 4$	1.7e-08→ 3.8e-01
cbms1	11	1	$0 \rightarrow 4$	4.2e-05→ 5.0e-01
cbms2	8	1	$0 \rightarrow 4$	1.2e-08→ 5.0e-01
mth191	4	1	$1 \rightarrow 4$	1.3e-08→ 3.5e-02
decker1	3	2	$1 \rightarrow 3 \rightarrow 8$	3.4e-10→ 2.6e-02
decker2	4	3	$1 \rightarrow 3 \rightarrow 7 \rightarrow 16$	4.5e-13→ 6.9e-03
decker3	2	1	$1 \rightarrow 4$	4.6e-08→ 2.5e-02
ojika1	3	2	$1 \rightarrow 3 \rightarrow 8$	9.3e-12→ 4.3e-02
ojika2	2	1	$2 \rightarrow 6$	3.3e-08→ 7.4e-02
ojika3	4	1	$1 \rightarrow 5$	6.5e-08→ 8.0e-02
ojika4	3	2	$2 \rightarrow 5 \rightarrow 12$	1.9e-13→ 2.4e-04
cyclic9	4	1	$7 \rightarrow 17$	5.6e-10→ 1.8e-03

There are 5,594 (333 orbits of size 18) isolated regular cyclic 9-roots, in addition to the 162 isolated solutions of multiplicity four. One deflation suffices to restore quadratic convergence on all 162 quadruple roots of this large application.

6. Conclusion

Our modified deflation method has plusses and minuses:

+ effective, numerically stable, relatively simple to implement; and
+ encouraging wide class of examples tested successfully; but...
– more theoretical insight is needed; and moreover:
– the doubling of the number of equations may lead to huge systems.

Future work will include the use of Puiseux series, see [4] and [5].

More References

[4] B. Huber and J. Verschelde. **Polyhedral end games for polynomial continuation.** *Numerical Algorithms*, 18(1):91–108, 1998.

[5] G. Lecerf. **Quadratic Newton Iteration for Systems with Multiplicity** *Found. Comput. Math.* 2:247–293 2002.

[6] J. Verschelde. **Algorithm 795: PHCpack: A general-purpose solver for polynomial systems by homotopy continuation.** *ACM Trans. Math. Softw.*, 25(2):251–276, 1999. Available at `http://www.math.uic.edu/~jan`.