

Locating the Closest Singularity in a Polynomial Homotopy

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Abstract. A polynomial homotopy is a family of polynomial systems, where the systems in the family depend on one parameter. If for one value of the parameter we know a regular solution, then what is the nearest value of the parameter for which the solution in the polynomial homotopy is singular? For this problem we apply the ratio theorem of Fabry. Richardson extrapolation is effective to accelerate the convergence of the ratios of the coefficients of the series expansions of the solution paths defined by the homotopy. For numerical stability, we recondition the homotopy. To compute the coefficients of the series we propose the quaternion Fourier transform. We locate the closest singularity computing at a regular solution, avoiding numerical difficulties near a singularity.

Keywords: Analytic continuation · Asymptotic expansion · Richardson extrapolation · Fabry · Fourier · Polynomial homotopy · Quaternion Taylor series · Singularity

1 Introduction

Polynomial homotopies define the deformation of polynomial systems, from systems with known solutions into systems that must be solved. We call a solution regular if the matrix of all partial derivatives evaluated at the solution has full rank, otherwise the solution is *singular*. We aim to locate the nearest singularity starting at a regular solution. Applying the ratio theorem of Fabry, we can detect singular points based on the coefficients of the Taylor series.

Theorem 1 (the ratio theorem of Fabry [11]). If for the series $x(t) = c_0 + c_1 t + c_2 t^2 + \dots + c_n t^n + c_{n+1} t^{n+1} + \dots$, we have $\lim_{n \to \infty} c_n/c_{n+1} = z$, then

- z is a singular point of the series, and
- it lies on the boundary of the circle of convergence of the series.

Then the radius of this circle is less than |z|.

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While the proof of the theorem would take us deep into complex analysis [9, Chapter XI], one can immediately verify that the ratio c_n/c_{n+1} is the pole of Padé approximants ([1,38]) of degrees [n/1], where n is the degree of the numerator, with linear denominator.

The ratio theorem of Fabry provides a radar to detect singularities in an adaptive step size control for continuation methods, as introduced in [39] (with a parallel implementation in [40]) and reproduced by [41]. Earlier applications of Padé approximants in deformation methods appeared in [20], in a symbolic context, and in [35] in a numerical setting. Empirically, in the plain application of this ratio theorem, already relatively few terms in the series appear to be sufficient to take nearby singularities into account.

The problem considered in this paper can be stated as follows. How many terms in the Taylor series do we need to locate the closest singularity with eight decimal places of accuracy? Answering this question exactly is not possible because of constants which differ for each series, but we can provide information about the order of the number of terms, e.g.: tens or hundreds.

We show that Richardson extrapolation (see [3] for a general formalism) effectively solves our problem. On monomial homotopies (defined in the next section), we can separate our problem from the required accuracy of the coefficients of the Taylor series. On examples, at 64 terms of the series, we obtain eight decimal places of accuracy in the location of the radius of convergence. In the third section, the justification for this successful application of Richardson extrapolation is proven. This is the first contribution of this paper.

The second contribution of this paper is the introduction of the quaternion Fourier transform [10,34] to compute the coefficients of the series. If we want to locate a singularity to full double precision, then, on examples, it appears that 512 terms in the series are needed. The Fast Fourier Transform scales well.

In the fifth section, we consider the application of Richardson extrapolation in an end game, when the path tracker approaches an isolated singular solution at the end of the path. Power series methods for singular solutions in [28] introduced the concept of the end game operation range. In this range, the continuation parameter has values for which the Puiseux series expansions are valid and where the numerical condition numbers still allow to compute sufficiently accurate approximations of the points on the path. In fixed precision, this range may be empty. Using multiple double precision for ill-conditioned problems is wasteful due to the slow convergence of Newton's method. For homotopies with a random complex gamma constant, we introduce the notion of the last pole. With this last pole, we recondition the homotopy with a shift and stretch transformation.

The new methods are illustrated in section six. Deflation restores the quadratic convergence of Newton's method for an isolated singular solution, of multiplicity μ . While [25] proves that μ is the upper bound on the number of deflation steps, the numerical decision to apply deflation is left to a singular value decomposition of the Jacobian matrix, which may not always be reliable enough. Although deflation has been addressed by many (e.g. [4,5,7,8,15–17,26,27,30]), the question on when to deflate is an open problem.

2 Monomial Homotopies

The examples of the homotopies in this section have only one singularity.

A monomial homotopy is defined by an exponent matrix $A \in \mathbb{Z}^{n \times n}$ and an n-dimensional coefficient vector $\mathbf{c}(t)$ of invertible power series:

$$\mathbf{h}(\mathbf{x},t) = \mathbf{x}^A - \mathbf{c}(t) = \mathbf{0},\tag{1}$$

with $\mathbf{x} = (x_1, x_2, \dots, x_n)$, and the multi-index notation

$$\mathbf{a}_{i} = (a_{1,j}, a_{2,j}, \dots, a_{n,j}), \quad \mathbf{x}^{\mathbf{a}_{j}} = x_{1}^{a_{1,j}} x_{2}^{a_{2,j}} \cdots x_{n}^{a_{n,j}},$$
 (2)

where \mathbf{a}_{i} is the jth column of the matrix A.

For any specific value for t, the system $\mathbf{h}(\mathbf{x},t) = \mathbf{0}$ reduces to a system with exactly two monomials in every equation. The solving of such a system happens via a unimodular coordinate transformation defined by the Hermite normal form of A. Singular solutions can occur only when $\mathbf{c}(t) = \mathbf{0}$, only for specific values of t. While monomial homotopies have thus no direct practical use, they provide good test cases to experiment with algorithms and to introduce new ideas.

2.1 A Square Root Homotopy

The simplest example of a monomial homotopy is

$$x^2 - 1 + t = 0$$
, with solution $x(t) = \pm \sqrt{1 - t}$. (3)

The two paths defined by this homotopy are shown in Fig. 1.

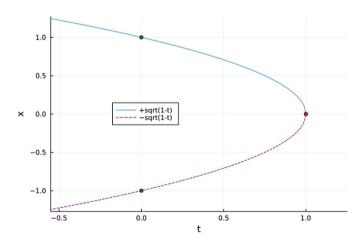


Fig. 1. Starting at $x = \pm 1$, the two paths converge to x = 0, as t moves from 0 to 1.

At t = 1, the two paths coincide at a double point. Our problem is to predict for which value of t this singularity happens without computing x(t) for $t \approx 1$.

In the development of the solution $x(t) = \sqrt{1-t}$ in a Taylor series about t = 0, let c_n be the coefficient of t^n . Then the application of the ratio theorem of Fabry gives

$$\frac{c_n}{c_{n+1}} = \frac{2(n+1)}{2n-1} =: f(n), \quad \lim_{n \to \infty} f(n) = 1.$$
 (4)

As the limit of the ratios equals one, we can predict the location of the singularity, already at the series development at t = 0. The main problem is the slow convergence of the series. Table 1 illustrates that in order to gain one extra bit of accuracy, we must double the value of n.

Table 1. $f(n) = \frac{2(n+1)}{2n-1}$ converges slowly to one. The error column lists |f(n)-1|. The last column is the ratio of two consecutive errors. As n doubles, the error is cut in half.

n	f(n)	error	error ratio
2	2.0000000000000000	1.00E+00	
4	1.42857142857143	4.29E - 01	2.3333E+00
8	1.2000000000000000	2.00E-01	2.1429E+00
16	1.09677419354839	9.68E - 02	2.0667E+00
32	1.04761904761905	4.76E - 02	2.0323E+00
64	1.02362204724409	2.36E - 02	2.0159E+00
128	1.01176470588235	1.18E - 02	2.0079E+00
256	1.00587084148728	5.87E - 03	2.0039E+00
512	1.00293255131965	2.93E - 03	2.0020E+00

Observe we can rewrite f(n) of (4) as

$$f(n) = \frac{2(n+1)}{2n-1} = \frac{2n-1+3}{2n-1} = 1 + \frac{3}{2n-1} = 1 + \frac{3}{2n} \left(\frac{1}{1-\frac{1}{2n}}\right)$$
 (5)

$$= 1 + \frac{3}{2n} \left(1 + \frac{1}{2n} + \left(\frac{1}{2n} \right)^2 + \left(\frac{1}{2n} \right)^3 + \cdots \right). \tag{6}$$

As shown in Sect. 3, f(n) has an asymptotic expansion of the form

$$f(n) = 1 + \gamma_1 \left(\frac{1}{n}\right) + \gamma_2 \left(\frac{1}{n}\right)^2 + \gamma_3 \left(\frac{1}{n}\right)^3 + \cdots$$
 (7)

for some coefficients $\gamma_1, \gamma_2, \gamma_3, \ldots$ If we double the value for n, we have

$$f(2n) = 1 + \gamma_1 \left(\frac{1}{2n}\right) + \gamma_2 \left(\frac{1}{2n}\right)^2 + \gamma_3 \left(\frac{1}{2n}\right)^3 + \cdots$$
 (8)

and then we eliminate γ_1 via a linear combination:

$$2f(2n) - f(n) = 1 + 2\gamma_2 \left(\frac{1}{2n}\right)^2 - \gamma_2 \left(\frac{1}{n}\right)^2 + 2\gamma_3 \left(\frac{1}{2n}\right)^3 - \gamma_3 \left(\frac{1}{n}\right)^3 + \cdots, (9)$$

which results in an approximation with error $O(1/n^2)$.

This regular ratio of two consecutive errors allows for an effective application of Richardson extrapolation. The input to Richardson extrapolation are the values $f(2), f(4), f(8), \ldots, f(2^N)$. The output is $R_{i,j}$, the triangular table of extrapolated values. Then the extrapolation proceeds as follows:

- 1. The first column: $R_{i,1} = f(2^i)$, for i = 1, 2, 3, ..., N.
- 2. The next columns in the table are computed via

$$R_{i,j} = \frac{2^{i-j+1}R_{i,j-1} - R_{j-1,j-1}}{2^{i-j+1} - 1},$$
(10)

for
$$i = i, i + 1, ..., N$$
 and for $j = 2, 3, ..., N$.

Table 2 shows the errors $|R_{i,j}-1|$ of the extrapolated values. Looking at the diagonal of Table 2, we see that we gain about two decimal places of accuracy at each doubling of n.

Table 2. Errors of Richardson extrapolation. The column E_0 is the error column of Table 1. The column E_j is the error obtained from extrapolating j times, applying formula (10). At n = 64 we have 8 correct decimal places and at n = 512, the full machine precision is attained.

n	E_0	E_1	E_2	E_3	E_4	E_5	E_6	E_7	E_8
2	1.0E+0								
4	4.3E - 1	1.4E - 1							
8	2.0E - 1	6.7E - 2	9.5E - 3						
16	9.7E - 2	3.2E-2	4.6E - 3	3.1E - 4					
32	4.8E - 2	1.6E - 2	2.3E - 3	1.5E-4	4.9E - 6				
64	2.4E - 2	7.9E - 3	1.1E - 3	7.5E - 5	2.4E-6	3.8E - 8			
128	1.2E - 2	3.9E - 3	5.6E - 4	3.7E - 5	1.2E - 6	1.9E - 8	1.5E - 10		
256	5.9E - 3	2.0E - 3	2.8E - 4	1.9E - 5	6.0E - 7	9.5E - 9	7.5E - 11	2.9E - 13	
512	2.9E - 3	9.8E - 4	1.4E - 4	9.3E-6	3.0E - 7	4.8E-9	3.8E - 11	1.5E - 13	4.4E - 16

2.2 Two Paths Ending in a Cusp

Figure 2 is an example of a situation not covered by Theorem 1. Consider the homotopy

$$h(x,t) = x^2 - (t-1)^4 = (x - (t-1)^2)(x + (t-1)^2) = 0,$$
(11)

which has the obvious two solutions $x(t) = \pm (t-1)^2$.

In this case, the power series for both paths are polynomials of degree two, and there is no limit, as all coefficients $c_n = 0$, for n > 2. In [32], an algorithm to sweep an algebraic curve for singularities monitors the determinant of the Jacobian matrix along the curve. If the path of the determinant of the Jacobian matrix on the curve is concave up, then that is an indicator for undetected singularities.

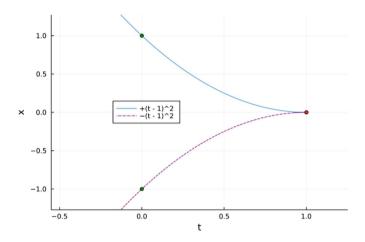


Fig. 2. Starting at $x = \pm 1$, the two paths converge to x = 0, as t moves from 0 to 1.

2.3 A Random 4-Dimensional Monomial Homotopy

In this section, we illustrate the need for multiple precision, even already in relatively low dimensions and degrees. Consider

$$\mathbf{h}(\mathbf{x},t) = \begin{cases} x_1^7 x_2^7 x_3^7 x_4^7 = 1 - t, \\ x_1^7 x_2^3 x_3^2 = 1 - t, \\ x_2^5 x_3 x_4 = 1 - t, \\ x_2^7 x_3^2 x_4^2 = 1 - t. \end{cases}$$
(12)

Storing the exponents of the monomials in the columns of $A = [\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{a}_4], \mathbf{x}^A = (\mathbf{x}^{\mathbf{a}_1}, \mathbf{x}^{\mathbf{a}_2}, \mathbf{x}^{\mathbf{a}_3}, \mathbf{x}^{\mathbf{a}_4}),$ the monomial homotopy $\mathbf{h}(\mathbf{x}, t)$ can be written as

$$\mathbf{x}^{A} = (1 - t)\mathbf{e}, \quad \mathbf{e} = \begin{bmatrix} 1\\1\\1\\1 \end{bmatrix}, \quad A = \begin{bmatrix} 7 & 7 & 0 & 0\\7 & 3 & 5 & 7\\7 & 2 & 1 & 2\\7 & 0 & 1 & 2 \end{bmatrix}, \quad \det(A) = -42.$$
 (13)

At t = 0, (1,1,1,1) is one of the 42 solutions, as $42 = |\det(A)|$, computed via the Smith normal form of A.

In double precision, extrapolating on $x_1(t)$, the extrapolation does not get any more accurate than six decimal places. Working with coefficients computed with 32 decimal places running the algorithms of [2] (implemented in PHCpack [42]), the extrapolation gives eight decimal places of accuracy, similarly as in the square root homotopy.

For the examples in this section, Richardson extrapolation results in an accuracy of 8 decimal places when n=64 and for n=512, we can locate to singularity to the full double precision.

3 Asymptotic Expansions

Consider the coefficient c_n of t^n in the Taylor series. What happens if n grows:

$$\left| \frac{c_n}{c_{n+1}} \right| \to \begin{cases} |z| < 1 : \text{coefficients increase,} \\ |z| = 1 : \text{coefficients are constant,} \\ |z| > 1 : \text{coefficients decrease.} \end{cases}$$
 (14)

Let x(t) satisfy h(x(t),t) = 0, then in the series for x(t), we may assume that for sufficiently large n, the magnitude of the nth coefficient is $|z|^n$. If we then set

$$t = |z|s \tag{15}$$

then the coefficient of s^n in the series x(s) will have a magnitude close to one. By Lemma 1, the radius of convergence of the series x(s) equals one.

Lemma 1. Let x(t) be a power series with c_n as the nth coefficient of t^n and

$$\lim_{n \to \infty} \frac{c_n}{c_{n+1}} = z \in \mathbb{C} \setminus \{0\}. \tag{16}$$

Then the series x(t = |z|s) has convergence radius equal to one.

Proof. Consider the effect of the substitution t = |z|s, respectively on the nth and the (n + 1)th term in the series x(t):

$$c_n t^n \to \underbrace{c_n |z|^n}_{=: d_n} s^n, \quad c_{n+1} t^{n+1} \to \underbrace{c_{n+1} |z|^{n+1}}_{=: d_{n+1}} s^{n+1}.$$
 (17)

Then d_n is the coefficient of s^n in the series x(s) and

$$\left| \frac{d_n}{d_{n+1}} \right| = \left| \frac{c_n}{c_{n+1}} \right| \frac{1}{|z|}.$$

By (16), $\lim_{n\to\infty} \left| \frac{d_n}{d_{n+1}} \right| = 1$. Thus, x(s) has a convergence radius equal to one. \square

If interested only in the magnitude of the radius, then in the natural application of Lemma (15), |z| is used. Using complex arithmetic, the series $x(t = z \cdot s)$ has radius of convergence equal to one.

In practice, the transformation as defined in as defined in (15) has numerical benefits. In theory, it implies that without loss of generality, we may assume that all series we consider all have convergence radius one.

Proposition 1. Assume x(t) is a series which satisfies the conditions of Theorem 1, with a radius of convergence equal to one. Let c_n be the coefficient of t^n in the series. Then $|1 - c_n/c_{n+1}|$ is O(1/n) for sufficiently large n.

Proof. Expressing the Taylor series of x(t) as

$$x(t) = x(0) + x'(0)t + \frac{x''(0)}{2!}t^2 + \frac{x'''(0)}{3!}t^3 + \dots + \frac{x^{(n)}(0)}{n!}t^n + \dots$$
 (18)

leads to a formula for the coefficient of t^n as

$$c_n = \frac{x^{(n)}(0)}{n!}$$
 and $c_{n+1} = \frac{x^{(n+1)}(0)}{(n+1)!}$. (19)

Then the error is

$$\left| 1 - \frac{c_n}{c_{n+1}} \right| = \left| 1 - \left(\frac{x^{(n)}(0)}{x^{(n+1)}(0)} \right) (n+1) \right| \approx 0, \quad \text{for large } n.$$
 (20)

Under the assumption that the radius of convergence is equal to one, without loss of generality we may assume that the singularity occurs at t=1. Otherwise, if t=z for some complex number z, with |z|=1, we can rotate the coordinate system so z=1 in the rotated coordinate system. Therefore, we may assume there is a power series p(t), so

$$x(t) = \frac{p(t)}{1-t} = u(t)p(t), \quad u(t) = \frac{1}{1-t} = 1 + t + t^2 + t^3 + \cdots$$
 (21)

The p(t)/(1-t) can be viewed as the limit of the Padé approximant of degree [n/1], for $n \to \infty$. This Padé approximant is well defined under the assumption of Theorem 1. In the limit reasoning for $n \to \infty$, we work with sufficiently large n, but never take ∞ for n.

Applying Leibniz rule to the nth derivative of x(t) leads to

$$x^{(n)}(t) = \sum_{k=0}^{n} \left(\frac{n!}{k!(n-k)!} \right) u^{(n-k)}(t) p^{(k)}(t).$$
 (22)

At t = 0, we have $u^{(n-k)}(0) = (n-k)!$ and we obtain

$$x^{(n)}(0) = \sum_{k=0}^{n} \left(\frac{n!}{k!}\right) p^{(k)}(0).$$
 (23)

We rewrite the expression for $x^{(n+1)}(0)$ as

$$x^{(n+1)}(0) = \sum_{k=0}^{n+1} \left(\frac{(n+1)!}{k!} \right) p^{(k)}(0)$$
 (24)

$$= \sum_{k=0}^{n} (n+1) \left(\frac{n!}{k!}\right) p^{(k)}(0) + p^{(n+1)}(0)$$
 (25)

$$= (n+1)x^{(n)}(0) + p^{(n+1)}(0).$$
(26)

Then we can write (20) as

$$\left| 1 - \frac{c_n}{c_{n+1}} \right| = \left| 1 - \left(\frac{x^{(n)}(0)}{(n+1)x^{(n)}(0) + p^{(n+1)}(0)} \right) (n+1) \right| \qquad (27)$$

$$= \left| 1 - \frac{1}{1 + \frac{1}{n+1} \left(\frac{p^{(n+1)}(0)}{x^{(n)}(0)} \right)} \right|. \qquad (28)$$

Note that we may divide by $x^{(n)}(0)$, because $x^{(n)}(0) \neq 0$ by the assumption that c_n/c_{n+1} is well defined for all values of n, otherwise the limit would not exist. Denote

$$C = \frac{p^{(n+1)}(0)}{x^{(n)}(0)}. (29)$$

Then the result follows from another series expansion:

$$\frac{1}{1 + \frac{C}{n+1}} = 1 - \left(\frac{C}{n+1}\right) + \left(\frac{C}{n+1}\right)^2 - \dots$$
 (30)

Substituting the right hand side of (30) into (28) gives

$$\left|1 - \frac{c_n}{c_{n+1}}\right| = \left|\left(\frac{C}{n+1}\right) - \left(\frac{C}{n+1}\right)^2 + \cdots\right|$$
(31)

What remains to prove is that C does not depend on n. Dividing (26) by $x^{(n)}(0)$ leads to

$$\frac{x^{(n+1)}(0)}{x^{(n)}(0)} = n + 1 + \frac{p^{(n+1)}(0)}{x^{(n)}(0)}.$$
(32)

The assumption that x(t) has a radius of convergence equal to one implies $c_{n+1} \approx c_n$ and that

$$\frac{x^{(n+1)}(0)}{x^{(n)}(0)} = n + O(1), \tag{33}$$

and thus we have

$$n + O(1) = n + 1 + \frac{p^{(n+1)}(0)}{x^{(n)}(0)}$$
 or equivalently $\frac{p^{(n+1)}(0)}{x^{(n)}(0)}$ is $O(1)$. (34)

Therefore C is a constant, independently of n. This shows that the error is O(1/(n+1)). For large n, O(1/(n+1)) is O(1/n).

Observe that the above proof does not make any assumptions on the type of homotopy used, other than the existence of a limit as in the theorem of Fabry. Then the main result of this section can be stated as below.

Corollary 1. Assuming the convergence radius equals one, applying Richardson extrapolation N times on a Taylor series truncated after n terms, results in an $O(1/n^{N+1})$ error on the radius of convergence.

Proof. By Proposition 1, and in particular the expansion in (31), we have

$$1 + \gamma_1 \left(\frac{1}{n}\right) + \gamma_2 \left(\frac{1}{n}\right)^2 + \gamma_3 \left(\frac{1}{n}\right)^3 + \cdots$$
 (35)

as the expansion for the error to the limit 1.

For N=1, the first extrapolated values have error $O(1/n^2)$, because the leading terms of the errors are O(1/n) and running Richardson extrapolation once (for j=2 and $i=2,3,\ldots,N$ in (10)) eliminates this leading term.

Using the formulas in (10) to compute the next columns in the triangular table eliminates the next terms in the error expansion in (35). After extrapolating N-1 more times, we then obtain an $O(1/n^{N+1})$ error term.

The assumption that the radius of convergence equals one makes the Richardson extrapolation superfluous, as the outcome of the extrapolation is already known. We can remove this assumption. Consider for example the homotopy $h(x,t)=x^2-2+t=0$ and $x(t)=\sqrt{2-t}$ as the positive solution branch. If c_n is the nth coefficient of the Taylor series, then

$$\frac{c_n}{c_{n+1}} = 2\left(\frac{2(n+1)}{2n-1}\right) = 2f(n),\tag{36}$$

where f(n) is the formula from (4). Similarly, for the homotopy $h(x,t) = x^2 - 1/2 + t = 0$ and $x(t) = \sqrt{1/2 - t}$ as the positive solution branch, with c_n as the nth coefficient of the Taylor series, we have

$$\frac{c_n}{c_{n+1}} = \frac{1}{2} \left(\frac{2(n+1)}{2n-1} \right) = \frac{1}{2} f(n). \tag{37}$$

This implies that for those two examples, the series development of f(n) in 1/n is multiplied respectively with 2 or 1/2, and that therefore Richardson extrapolation applies.

Theorem 2. Let c_n be the coefficient with t^n in x(t) and denote $f(n) = c_n/c_{n+1}$. If

$$\lim_{n \to \infty} \frac{c_n}{c_{n+1}} = z \in \mathbb{C} \setminus \{0\},\tag{38}$$

then

$$f(n) = z + \gamma_1 z \left(\frac{1}{n}\right) + \gamma_2 z \left(\frac{1}{n}\right)^2 + \gamma_3 z \left(\frac{1}{n}\right)^3 + \cdots$$
 (39)

Proof. By Lemma 1, we transform x(t) into $x(s) = x(t = z \cdot s)$, which has convergence radius one. Let d_n be the coefficient of s^n in x(s) and denote $g(n) = d_n/d_{n+1}$. For g(n), we have the expansion (35):

$$g(n) = 1 + \gamma_1 \left(\frac{1}{n}\right) + \gamma_2 \left(\frac{1}{n}\right)^2 + \gamma_3 \left(\frac{1}{n}\right)^3 + \cdots$$
 (40)

The above series development is unique. Therefore, transforming s = t/z, gives the series (39).

Theorem 2 provides the justification for the application of Richardson extrapolation and the statement of Corollary 1 holds in theory for any series, not only for those with radius of convergence equal to one. However, in practice, series with a radius of convergence smaller than one will have very large coefficients which cause numerical instabilities and unavoidably arithmetical overflow.

If the convergence radius of a power series equals one, then it is safe to calculate the coefficients of the power series from sample points at nearby locations.

4 Fourier Series

In computational complex analysis [18], the discrete Fourier transform is applied to compute the coefficients of the Taylor series. For general references on the application of Fourier transforms in computer algebra and numerical analysis, we refer to [14] and [6].

As described in [29], many derivatives are computed simultaneously with an accuracy close to machine precision, for a suitable step size, using complex arithmetic, extending the complex-step differentiation method [37] to higher order derivatives. Figure 3 illustrates the problem: the step size must be smaller than the radius of convergence. This problem is addressed in Sect. 5.2.

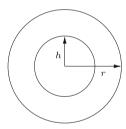


Fig. 3. The radius of convergence r and step size h. We want $h \ll r$.

To introduce the application of the discrete Fourier transform to compute the Taylor series, consider the development of f at z, using step size $h\omega$:

$$f(z+h\omega) = f(z) + h\omega f'(z) + \frac{h^2}{2}\omega^2 f''(z) + \frac{h^3}{3!}\omega^3 f'''(z)$$

$$+ \frac{h^4}{4!}\omega^4 f^{(iv)}(z) + \frac{h^5}{5!}\omega^5 f^{(v)}(z) + \frac{h^6}{6!}\omega^6 f^{(vi)}(z)$$

$$+ \frac{h^7}{7!}\omega^7 f^{(vii)}(z) + \frac{h^8}{8!}\omega^8 f^{(viii)}(z) + \cdots,$$

where ω is the eight complex root of unity: $\omega^8 = 1$. Regrouping in powers of ω then gives

$$f(z + h\omega) = f(z) + \frac{h^8}{8!} f^{(\text{viii})}(z) + \cdots$$

$$+ \omega \left(hf'(z) + \frac{h^9}{9!} f^{(\text{ix})}(z) + \cdots \right)$$

$$+ \omega^2 \left(\frac{h^2}{2!} f''(z) + \frac{h^{10}}{10!} f^{(\text{x})}(z) + \cdots \right)$$

$$+ \omega^3 \left(\frac{h^3}{3!} f'''(z) + \frac{h^{11}}{11!} f^{(\text{xii})}(z) + \cdots \right)$$

$$+ \omega^4 \left(\frac{h^4}{4!} f^{(\text{iv})}(z) + \frac{h^{12}}{12!} f^{(\text{xiii})}(z) + \cdots \right)$$

$$+ \omega^5 \left(\frac{h^5}{5!} f^{(\text{v})}(z) + \frac{h^{13}}{13!} f^{(\text{xiii})}(z) + \cdots \right)$$

$$+ \omega^6 \left(\frac{h^6}{6!} f^{(\text{vi})}(z) + \frac{h^{14}}{14!} f^{(\text{xiv})}(z) + \cdots \right)$$

$$+ \omega^7 \left(\frac{h^7}{7!} f^{(\text{vii})}(z) + \frac{h^{15}}{15!} f^{(\text{xv})}(z) + \cdots \right).$$

For k from 1 to 7, the coefficients of ω^k allow the extraction of the kth derivative of f at z, at a precision of $O(h^8)$.

The Discrete Fourier Transform

$$DFT_{\omega}: \mathbb{C}^{n} \to \mathbb{C}^{n} (f_{0}, f_{1}, \dots, f_{n-1}) \mapsto (F(\omega^{0}), F(\omega^{1}), \dots, F(\omega^{n-1}))$$

$$(41)$$

takes the coefficients of the polynomial F with coefficients $f_0, f_1, \ldots, f_{n-1}$, where $\omega^n = 1$ and returns the values of F at the powers of ω . The inverse of DFT $_\omega$ returns the coefficients of ω^k needed in the Taylor series of $f(z + h\omega)$.

As illustrated by Table 3, the derivatives grow as fast as n! and therefore, except for small n, we may not expect to obtain highly accurate values.

The step size of h = 0.5 used in Table 3 is a compromise value. Values of h smaller than 0.5 give more accurate results for the lower order derivatives but give then too inaccurate values for the higher order derivatives. The opposite happens for values of h larger than 0.5.

Fortunately, we do not need the derivatives $x^{(n)}(0)$, but the coefficients of the Taylor series, $c_n = x^{(n)}(0)/n!$. Table 4 shows the application of the DFT to compute the series coefficients. Compared to the derivatives in Table 3, the computations in double precision arithmetic give six decimal places of accuracy for n = 64. The step size h = 0.85 gave the most accurate results.

In machine double precision, the results in Table 3 and Table 4 are close to optimal, with the step sizes respectively equal to 0.5 and 0.85. Using those large step sizes in multiprecision will not give more accurate results, but multiprecision will allow to select smaller step sizes. In particular with 33 decimal places (using

n	exact $x^{(n)}(0)$	approximation $x^{(n)}(0)$	error
0	1.000000000000	0.99999968596	3.14E - 08
1	-0.500000000000	-0.500000028787	5.76E - 08
2	-0.2500000000000	-0.250000053029	2.12E - 07
3	-0.3750000000000	-0.375000147155	3.92E - 07
4	-0.937500000000	-0.937500546575	5.83E - 07
5	-3.281250000000	-3.281252546540	7.76E - 07
6	-14.765625000000	-14.765639282757	9.67E - 07
7	-81.210937500000	-81.211031230822	1.15E - 06
8	-527.871093750000	-527.871798600561	$1.34E\!-\!06$
9	-3959.033203125000	-3959.039180858922	1.51E - 06
10	-33651.782226562500	-33651.838679975779	1.68E - 06
11	-319691.931152343750	-319692.518875707698	1.84E - 06
12	-3356765.277099609375	-3356771.966430745088	1.99E - 06
13	-38602800.686645507812	-38602883.297614447773	2.14E - 06
14	-482535008.583068847656	-482536106.155545711517	2.27E - 06
15	-6514222615.871429443359	-6514238371.741491317749	$2.42E\!-\!06$
16	-94456227930.135726928711	-94456466497.677398681641	2.53E-06

Table 3. Derivatives of $x(t) = \sqrt{1-t}$ at t=0. The approximate values are computed with step size h=0.5. The last column is the relative error.

mpmath 1.1.0 [21] with SymPy 1.4 [23] in Python 3.7.3), the 16th derivative is computed with an accuracy of 15 decimal places, with step size 0.1 and the error on the 64th coefficient coefficient on the series drops to 10^{-11} , with step size 0.5.

Instead of working with the same step size for all series coefficients, alternatively, one could explore using different step sizes. In this context, one classical and very common application of Richardson extrapolation is to improve the accuracy of numerical differentiation.

When z is a complex number, the complex step derivative is generalized in [24] and [33] with quaternion arithmetic. Using the quaternion Fourier transform [10,34], the coefficients of the Taylor series can be computed.

Table 4. Coefficients c_n of the Taylor series of $x(t) = \sqrt{1-t}$ at t=0. The approximate values are computed with step size h=0.85. The last column is the relative error.

n	exact c_n	approximation	error
0	1.0000000000000	0.999999986011	1.40E - 08
1	-0.5000000000000	-0.500000013671	2.73E - 08
2	-0.1250000000000	-0.125000013365	1.07E - 07
4	-0.039062500000	-0.039062512786	3.27E - 07
8	-0.013092041016	-0.013092052762	8.97E - 07
32	-0.001576932599	-0.001576940258	4.86E - 06
64	-0.000554221198	-0.000554226120	8.88E - 06

5 Polynomial Homotopies

The homotopies in this section have multiple singularities in the complex plane, for complex values of t, with real part < 1, but only one singularity at t = 1. Knowing the location of the last pole leads to the reconditioning of the homotopy and to series with convergence radius equal to one.

5.1 The Last Pole

Let $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ be the system we want to solve and assume we have at least one solution of $\mathbf{g}(\mathbf{x}) = \mathbf{0}$. Then the homotopy

$$\mathbf{h}(\mathbf{x}, t) = \gamma(1 - t)\mathbf{g}(\mathbf{x}) + t\mathbf{f}(\mathbf{x}) = \mathbf{0}, \quad t \in [0, 1], \quad \gamma \in \mathbb{C}, |\gamma| = 1, \tag{42}$$

defines a path starting at t = 0, at a solution of $\mathbf{g}(\mathbf{x}) = \mathbf{0}$ and ending at t = 1, at a solution of $\mathbf{f}(\mathbf{x}) = \mathbf{0}$. The constant γ is a random complex number. If $\mathbf{g}(\mathbf{x}) = \mathbf{0}$ has no singular solutions, then it follows from the main theorem of elimination theory that all paths defined by $\mathbf{h}(\mathbf{x}, t) = \mathbf{0}$ are regular and bounded for $t \in [0, 1)$, except for finitely many *complex* values for t. In [36], this constructive argument is illustrated by examples of homotopies of small degrees and dimension.

The key point is the existence of a polynomial H(t) of finite degree, with $H(0) \neq 0$, as $\mathbf{g}(\mathbf{x}) = \mathbf{0}$ has no singular solutions. Moreover, by the random complex choice of γ , all roots of H are in the complex plane, except for t = 1, if the system $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ has a singular solution. By construction of $\mathbf{h}(\mathbf{x}, t) = \mathbf{0}$, we can introduce the notion of the last pole, as the complex number ρ , for which $H(\rho) = 0$ and of all roots of H, ρ has the largest real part less than one.¹

Figure 4 illustrates that ρ is the last complex singular value detected by the radar of a path tracker which applies the theorem of Fabry to set its step size.

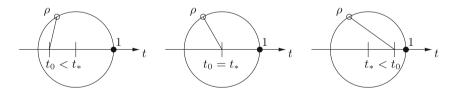


Fig. 4. Schematic of the last pole ρ marked by the hollow circle. At the center, at $t = t_0 = t_*$, ρ and 1 are at the same distance. At $t_0 < t_*$, the proximity of ρ determines the step size, while for $t_* < t_0$, the singularity at one will be detected.

By construction of the homotopy $\mathbf{h}(\mathbf{x},t) = \mathbf{0}$, and in particular by the random choice of the complex constant γ , the solution at $t = t_*$ is regular, and well conditioned. This implies that Newton's method for the series coefficients converges quadratically. One could then already discover the singular solution for

 $^{^{1}}$ If all real parts of the roots of H are larger than one, then we are in the case similar to a monomial homotopy, a case that is then already solved.

t=1, via the computation of a Padé approximant with quadratic denominator. Via a perturbation argument, for $t=t_*+\delta$, for suitable $\delta>0$, the application of the theorem of Fabry will detect t=1 as a singular solution, without computing $\mathbf{x}(t)$ for $t\approx 1$.

5.2 Homotopy Reconditioning

Once the path tracker reaches a value for the continuation parameter t, that is past the last pole towards an isolated singularity at t = 1, at the end of a path, the coefficients of the power series will grow very fast, which is already an indication for the trouble to come.

For the reliable numerical computation of the power series, consider the transformation in the homotopy $\mathbf{h}(\mathbf{x},t) = \mathbf{0}$:

$$t = rs + t_0, \quad r = 1 - t_0, \quad t_0 = t_* + \delta,$$
 (43)

where t_* is value as in Fig. 4, at the same distance from the last pole ρ and the end point t=1, and δ is a suitable positive value so at $t_0=t_*+\delta$, the application of the theorem of Fabry will detect t=1 as the location for the closest singular solution.

After applying (43), the series development of the path $\mathbf{x}(s)$ defined by the homotopy $\mathbf{h}(\mathbf{x}(s), s) = \mathbf{0}$ will have convergence radius equal to one. The term reconditioning is justified as the coefficients of the Taylor series in the reconditioned homotopy do not grow exponentially fast.

6 Computational Experiments

The new methods are illustrated with computational experiments on two well known examples in the literature, with ad hoc tools, using test procedures in version 2.4.85 PHCpack [42] (with QDlib [19] and CAMPARY [22] for multiple double arithmetic), version 1.1.1 of phcpy [31], version 1.4 of sympy [23], and version 1.1.0 of mpmath [21], in Python 3.7.3. The computations were done on a CentOS 6.10 Linux computer with 23.4 GB of memory and a 12-core Intel Xeon X5690 at 3.47 GHz.

6.1 Ojika's First Example

One example in [30] (known in benchmarks as ojika1, used in [16,25-27]) is

$$\mathbf{f}(x,y) = \begin{cases} x^2 + y - 3 = 0, \\ x + 0.125y^2 - 1.5 = 0. \end{cases}$$
(44)

This system has one regular solution at (-3,6) and a triple root at (1,2). Using $\gamma = -0.917153159675641 - 0.398534919043474 I, <math>I = \sqrt{-1}$, in the homotopy (42) with start system

$$\mathbf{g}(x,y) = \begin{cases} x^2 - 1 = 0, \\ y^2 - 1 = 0 \end{cases}$$
 (45)

makes that the path starting at (1, 1) converges to the triple root.

The value t_0 after t_* (the location of the last pole) that was used is $t_0 = 0.955647336181678$. At this value for t, the coordinates of the corresponding solution are

$$x \approx 1.17998166418735 + 0.0181391513338172 I,$$

 $y \approx 1.60871001974391 - 0.0423866308603763 I,$

with the inverse of the condition number estimated at 8.9E-03. In double precision, a condition number of about 10^3 is within the range of what is considered well conditioned. Observe that the coordinates of the solution corresponding to t_0 are far from the location of the triple root (1,2).

The value for $r = 1 - t_0$ is 0.044352663818322036, which implies that, without reconditioning, the magnitude of the Taylor series coefficients will increase with about two decimal places. At that pace, as $2^{64} \approx 10^{+19}$, numerical difficulties arise without reconditioning.

After reconditioning, with n = 64, the ratio, based on the power series for the first coordinate x(s), is estimated at

$$1.0265192231142901 + 2.9197227799819557E - 05I$$

and the magnitude of the imaginary part corresponds to the magnitude of the coefficients c_n in the series of x(s). This mild decline of the exponents corresponds to the over estimation of the radius at about 1.0265. Applying Richardson extrapolation yields

$$0.9999729580138075 + 8.484367218447337E - 06I$$

which thus locates the singularity with an error of 10^{-6} .

The above computations were done in double precision. In double precision (≈ 32 decimal places), with n=512, the ratio is first estimated at 1.00326 and Richardson extrapolation then improves the accuracy, to obtain an error of 10^{-6} on the value t=1, the location of the singularity, confirming the result obtained in double precision.

6.2 One Fourfold Root of Cyclic 9-Roots

The cyclic n-roots problem

$$\mathbf{f}(\mathbf{x}) = \begin{cases} x_0 + x_1 + \dots + x_{n-1} = 0\\ i = 2, 3, \dots, n-1 : \sum_{j=0}^{n-1} \prod_{k=j}^{j+i-1} x_{k \mod n} = 0\\ x_0 x_1 x_2 \cdots x_{n-1} - 1 = 0 \end{cases}$$
(46)

is a well known benchmark problem in polynomial system solving, which arose in the study of biunimodular vectors [13]. The cyclic 9-roots problem was solved in [12], and its roots of multiplicity four were used in the development of deflation

in [25]. This system was used to illustrate the computation of the multiplicity structure in [8].

The start system $\mathbf{g}(\mathbf{x}) = \mathbf{0}$ in a homotopy to solve $\mathbf{f}(\mathbf{x}) = \mathbf{0}$ was obtained by running the plain blackbox solver (the extended version is described in [43]) on 12 cores tracking 11,016 is less than two minutes. For reproducibility, the seed in the random number generators was 7131. That $\mathbf{g}(\mathbf{x})$ was then used in the homotopy (42) with $\gamma = -0.917153159675641 - 0.398534919043474 I, <math>I = \sqrt{-1}$. One path was selected that ended at one of the fourfold roots.

The value for t after t_* , the location of the last pole is $t_0 = 0.998315512784621$, with coordinates of the corresponding solution

```
\begin{array}{lll} x_0 \approx +1.00000126517819 & +2.90396442439194\mathrm{E}-07 \\ x_1 \approx -2.61867609654276 & -2.06312686218454\mathrm{E}-03 \\ x_2 \approx -0.381725080860952 + 6.25420054941098\mathrm{E}-05 \\ x_3 \approx +1.00151501674915 & +1.11189386260303\mathrm{E}-03 \\ x_4 \approx +0.381629266681896 - 3.62839287359460\mathrm{E}-04 \\ x_5 \approx +2.62034316800711 & +2.49236777820171\mathrm{E}-03 \\ x_6 \approx +0.998483898493147 - 1.11096857563447\mathrm{E}-03 \\ x_7 \approx -2.61970187995193 & -4.30339092688366\mathrm{E}-04 \\ x_8 \approx -0.381870388949536 + 3.01610075581641\mathrm{E}-04 \\ \end{array}
```

with inverse condition number estimated at 5.3E-5. Although the homotopy does not respect the permutation symmetry, the orbit structure of the solution can already be observed, at the limited accuracy of about three decimal places.

The value for $r = 1 - t_0$ is 0.0016844872153789492 and without reconditioning the homotopy, the coefficients in the power series expansions of the solution increase at a very high pace. After reconditioning, with n = 32, the convergence radius is estimated at

```
1.00000000099639 + 4.319265E - 09I
```

and confirmed in double precision. Because of the close proximity to the singularity, no extrapolation is necessary in this case.

7 Conclusions

Richardson extrapolation is effective to locate the closest singularity as shown by the asymptotic expansions on the ratio of two consecutive coefficients in the Taylor series of the solution curves, under the condition of the theorem of Fabry.

The homotopy continuation parameter can always be adjusted so the convergence radius of the power series equals one, which allows for a safe step size selection in the application of the discrete Fourier transform to compute all coefficients of the series efficiently and accurately.

Deflation restores the quadratic convergence of Newton's method on an isolated singular solution via reconditioning. The homotopy reconditioning using

the location of the last pole provides an apriori justification for the application of the deflation method via the Richardson extrapolation on the ratios of the coefficients of power series.

The theorem of Fabry provides a radar to detect singularities. In this paper we have shown that this radar can accurately locate the nearest singular solution of a polynomial homotopy. We apply this radar at a safe distance from singularities, at a regular solution where the quadratic convergence of Newton's method holds.

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