Extrapolating Towards Singular Solutions of Polynomial Homotopies (*preliminary report*)

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Extrapolating Towards Singular Solutions

problem statement

A polynomial homotopy is a family of polynomial systems, where the systems in the family depend on one parameter.

At a singular point, the matrix of all partial derivatives is not full rank.

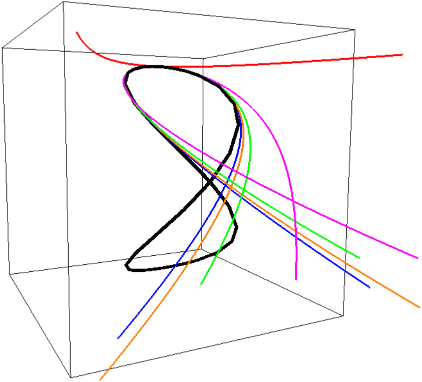
The *location problem* asks to detect the value of the parameter in the homotopy where a singular point occurs.

The *approximation problem* asks to accurately determine the coordinates of the singular point, once located.

We want an efficient and reliable criterion to decide whether singular points are *at infinity or not*.

power series developments of Viviani's curve

Viviani's curve expanded around $(0, 0, 2)$:



Looking at series of increasing orders, we observe their intersection as a predictor for the singular point where Viviani's curve intersects itself.

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detecting nearby singularities

Applying the ratio theorem of Fabry, we can detect singular points based on the coefficients of the Taylor series.

Theorem (the ratio theorem, Fabry 1896)

If for the series $x(t) = c_0 + c_1 t + c_2 t^2 + \cdots + c_n t^n + c_{n+1} t^{n+1} + \cdots$, *we have* $\lim\limits_{n \rightarrow \infty} c_n / c_{n+1} = z$, *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 $|z|$.

The ratio c_n / c_{n+1} is the pole of Padé approximants of degrees $[n/1]$ (n is the degree of the numerator, with linear denominator).

the ratio theorem of Fabry and Padé approximants

Consider $n = 3$, $x(t) = c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4$.

$$[3/1] = \frac{a_0 + a_1 t + a_2 t^2 + a_3 t^3}{1 + b_1 t}$$

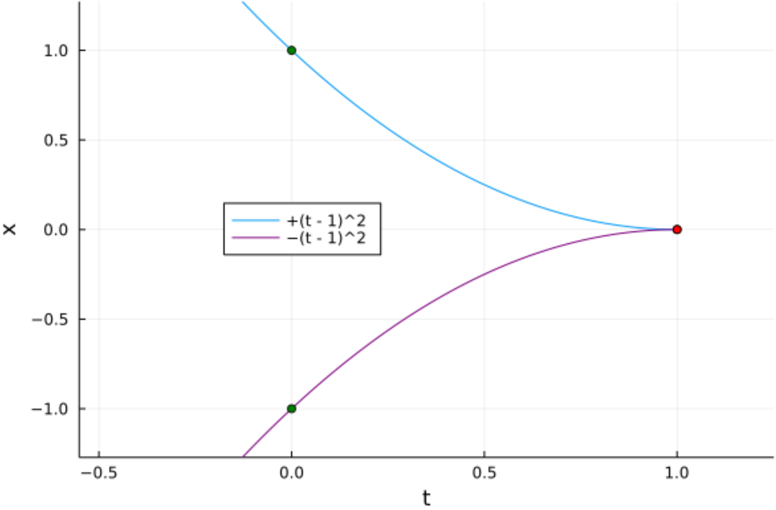
$$\begin{array}{rcl} (c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4)(1 + b_1 t) & = & a_0 + a_1 t + a_2 t^2 + a_3 t^3 \\ c_0 + \quad c_1 t + \quad c_2 t^2 + \quad c_3 t^3 + \quad c_4 t^4 & & \\ + b_1 c_0 t + b_1 c_1 t^2 + b_1 c_2 t^3 + b_1 c_3 t^4 & = & a_0 + a_1 t + a_2 t^2 + a_3 t^3 \end{array}$$

We solve for b_1 in the term for t^4: $c_4 + b_1 c_3 = 0 \Rightarrow b_1 = -c_4/c_3$.

The denominator of $[3/1]$ is $1 - c_4/c_3 t$. The pole of $[3/1]$ is c_3/c_4.

an example not covered by Fabry's theorem

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

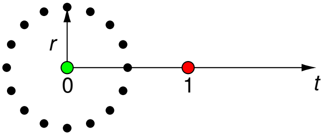


prior work

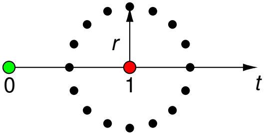
- N. Bliss and J. Verschelde. **The method of Gauss–Newton to compute power series solutions of polynomial homotopies.** *Linear Algebra and its Applications*, 542:569–588, 2018.
- S. Telen, M. Van Barel, and J. Verschelde. **A Robust Numerical Path Tracking Algorithm for Polynomial Homotopy Continuation.** *SIAM Journal on Scientific Computing* 42(6):A3610–A3637, 2020.
- J. Verschelde and Kylash Viswanathan. **Locating the Closest Singularity in a Polynomial Homotopy.** In the *Proceedings of the 24th International Workshop on Computer Algebra in Scientific Computing (CASC 2022)*, pages 333–352. Springer-Verlag, 2022.

difference with Cauchy integrals

- Use function values around the regular point at 0
  to compute the coefficients of the Taylor series:



- Use function values around the singularity at 1
  to compute the coefficients of the Laurent series:



In both cases, what is a good step size r?

numerical analytic continuation and extrapolation

- Peter Wynn. **The rational approximation of functions which are formally defined by a power series expansion.** *Math. Comp.* 14(70): 147–186, 1960.
- Peter Henrici. **An algorithm for analytic continuation.** *J. SIAM Numer. Anal.*, 3(1): 67–78, 1966.
- Peter Henrici. **Fast Fourier methods in computational complex analysis.** *SIAM Review*, 21(4):481–527, 1979.
- Bengt Fornberg. **Numerical differentiation of analytic functions.** *ACM TOMS*, 7(4):512–526, 1981.
- Claude Brezinski and Michela Redivo Zaglia. **Extrapolation Methods.** Elsevier, 1991.
- Avrim Sidi. **Practical Extrapolation Methods. Theory and Applications.** Cambridge University Press, 2003.

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Taylor series of roots of a polynomial homotopy

Consider the homotopy

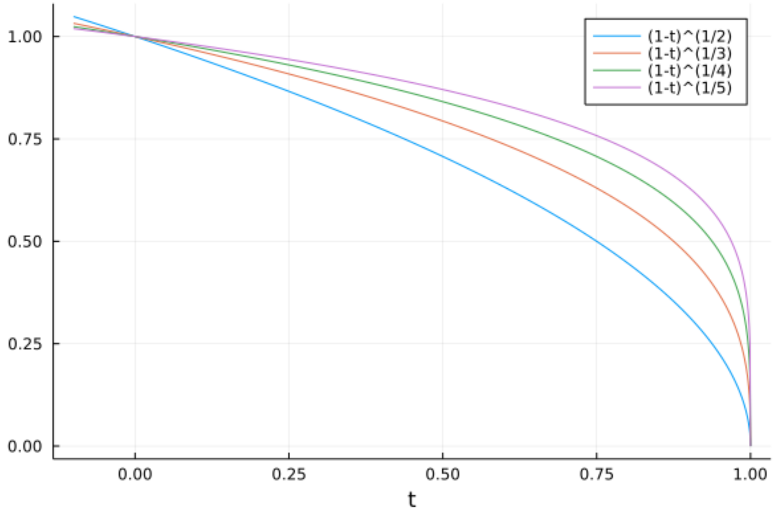
$$h(x,t) = x^2 - 1 + t = 0,$$

where x is the variable and t the parameter.

- At $t = 0$, the solutions are $x = \pm 1$.
- At $t = 1$, we have the double root $x = 0$.

In this test problem, starting at $t = 0$,
we compute 1 as the nearest singularity.

$x(t) = (1-t)^{1/\omega}$, $\omega = 2, 3, 4, 5$



testing for divergence

For testing, consider the monomial homotopy:

$$\begin{aligned} x^2 &= 1 - t, \\ x\,y &= 1. \end{aligned}$$

As $t \to 1$, $x(t) \to 0$ and $y(t) \to \infty$.

Apply the series of $\log(1-t) = -t - \dfrac{t^2}{2} - \dfrac{t^3}{3} - \dfrac{t^4}{4} + O(t^5)$
to the series for $x(t)$ and $y(t)$:

$$\begin{aligned} \log(1 - x(t)) &= -\frac{t}{2} - \frac{t^2}{4} - \frac{t^3}{6} - \frac{t^4}{8} + O(t^5), \\ \log(1 - y(t)) &= +\frac{t}{2} + \frac{t^2}{4} + \frac{t^3}{6} + \frac{t^4}{8} + O(t^5). \end{aligned}$$

The distinction between convergence and divergence can be made.

$\log(1 - x(t))$, for $x(t) = (1 - t)^{1/\omega}$, $\omega = 2, 3, 4, 5$

The expansions of $\log(1 - x(t))$:

$$
\begin{aligned}
\omega = 2 \quad &: \quad -\frac{t}{2} - \frac{t^2}{4} - \frac{t^3}{6} - \frac{t^4}{8} + O(t^5) \\
\omega = 3 \quad &: \quad -\frac{t}{3} - \frac{t^2}{6} - \frac{t^3}{9} - \frac{t^4}{12} + O(t^5) \\
\omega = 4 \quad &: \quad -\frac{t}{4} - \frac{t^2}{8} - \frac{t^3}{12} - \frac{t^4}{16} + O(t^5) \\
\omega = 5 \quad &: \quad -\frac{t}{5} - \frac{t^2}{10} - \frac{t^3}{15} - \frac{t^4}{20} + O(t^5)
\end{aligned}
$$

For $\log(1 - y(t))$ in $x^\omega = 1 - t$, $x\,y = 1$, flip signs.

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reduce to convergence radius one

Let c_n be the coefficient of t^n in the Taylor series.

Consider what happens if n grows:

$$\left| \frac{c_n}{c_{n+1}} \right| \rightarrow \left\{ \begin{array}{lcl} |z| < 1 & : & \text{coefficients increase,} \\ |z| = 1 & : & \text{coefficients are constant,} \\ |z| > 1 & : & \text{coefficients decrease.} \end{array} \right.$$

Lemma (reduction to convergence radius one, CASC 2022)

Let $x(t)$ be a power series with c_n as the coefficient of t^n and

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

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

convergence of the coefficient ratios

Proposition (convergence of the coefficient ratios, CASC 2022)

Assume $x(t)$ is a series which satisfies the conditions of the ratio theorem of Fabry, with a radius of convergence equal to one. Let c_n be the coefficient of t^n in the series, then

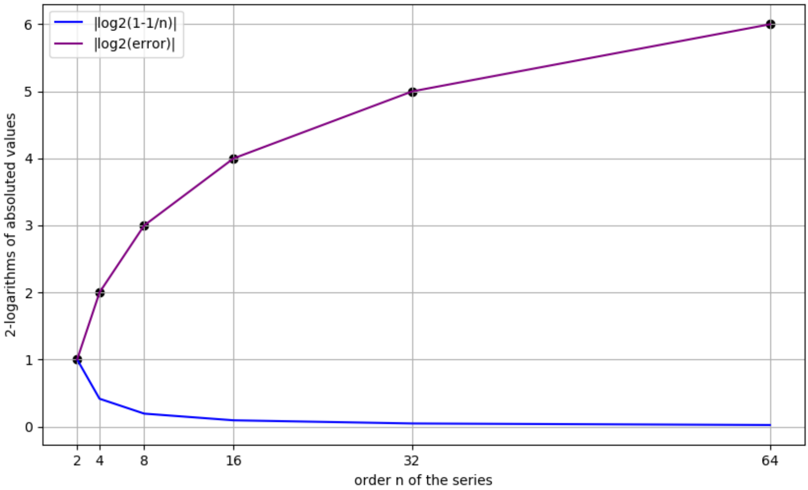
$$\left| 1 - \frac{c_n}{c_{n+1}} \right| \text{ is } O(1/n)$$

for sufficiently large n.

The good and the bad:

+ It confirms extensive computational experiments: using 8 terms of series are sufficient to avoid a singularity in the step size control.
− The $O(1/n)$ grows very slowly, e.g. $1/64 \approx 0.016$, $1/256 \approx 0.004$.

one extra bit of accuracy after each doubling of n



Richardson extrapolation

$$
\begin{aligned}
f(n) &= 1 + \gamma_1 \left(\frac{1}{n} \right) + \gamma_2 \left(\frac{1}{n} \right)^2 + \cdots \\
f(2n) &= 1 + \gamma_1 \left(\frac{1}{2n} \right) + \gamma_2 \left(\frac{1}{2n} \right)^2 + \cdots
\end{aligned}
$$

$$
\begin{aligned}
2f(2n) - f(n) &= 2 + 2\gamma_1 \left(\frac{1}{2n} \right) + 2\gamma_2 \left(\frac{1}{2n} \right)^2 + \cdots \\
&\quad -1 - \gamma_1 \left(\frac{1}{n} \right) - \gamma_2 \left(\frac{1}{n} \right)^2 - \cdots
\end{aligned}
$$

$$
2f(2n) - f(n) = 1 + \beta_2 \left(\frac{1}{n} \right)^2 + \cdots
$$

on the effectiveness of Richardson extrapolation

Input: $f(2)$, $f(4)$, $f(8)$, $\ldots$, $f(2^N)$.

Output: $T_{i,j}$, the triangular table of extrapolated values.

1. $T_{i,1} = f(2^i)$, for $i = 1, 2, 3, \ldots, N$.
2. For $j = i, i+1, \ldots, N$ and for $i = 2, 3, \ldots, N$:

$$T_{i,j} = \frac{2^i T_{i,j-1} - T_{1,j-1}}{2^i - 1}.$$

Corollary (Richardson extrapolation accelerates, CASC 2022)

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.

\+ With 64 terms, about 8 decimal places of accuracy are obtained.

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Aitken extrapolation

Given is a sequence **x** of n numbers, $\mathbf{x} = x_1, x_2, \ldots, x_n$.

Assume geometric convergence to the limit z with ratio r:

$$x_{k+1} - z = r(x_k - z), \quad |r| < 1.$$

Aitken extrapolation constructs a new sequence **y** of $n - 2$ numbers, using the formula

$$y_k = x_k - \frac{(x_{k+1} - x_k)^2}{x_{k+2} - 2x_{k+1} + x_k}, \quad k = 1, 2, \ldots, n - 2.$$

We apply this formula repeatedly, setting **y** to **x**,
for as long as $n \geq 2$.

repeated Aitken on $x(t) = (1-t)^{1/\omega}$, $\omega = 2, 3, 4, 5$

SymPy computes the Taylor series of $(1-t)^{1/\omega}$ up to order 64.
Let c_n be the coefficient with t^n, then

$$\frac{c_n}{c_{n+1}} \rightarrow R = 1 \quad \text{and} \quad \sum_{n=0}^{63} c_n \rightarrow S = 0.$$

Running Aitken repeatedly with exact rational arithmetic:

ω	error on R	error on S
2	2.29e-11	3.51e-07
3	2.02e-11	3.14e-05
4	1.89e-11	3.41e-04
5	1.81e-11	1.51e-03

Aitken is effective to locate and approximate the singularity,
ω has no effect on R, but its influence is observed on S.

Aitken for the convergence radius

Let c_n be the coefficient of t^n and assume $\lim_{n \to \infty} \left(\frac{c_n}{c_{n+1}} \right) = 1$.

To compute the ratio r in

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

substitute

$$\frac{c_n}{c_{n+1}} = 1 + \gamma_1 \left(\frac{1}{n} \right) + O\left(\frac{1}{n^2} \right), \quad \frac{c_{n+1}}{c_{n+2}} = 1 + \gamma_1 \left(\frac{1}{n+1} \right) + O\left(\frac{1}{n^2} \right),$$

which leads to

$$\gamma_1 \left(\frac{1}{n+1} \right) = r\, \gamma_1 \left(\frac{1}{n} \right) \quad \Rightarrow \quad r = \frac{n}{n+1} < 1.$$

geometric ratio for two consecutive terms

The ratio $r = r_n = \dfrac{n}{n+1}$ depends on n.

Consider:

$$\frac{n}{n+1} = 1 + \frac{n}{n+1} - 1 = 1 + \frac{n}{n+1} - \frac{n+1}{n+1} = 1 - \frac{1}{n+1}$$

and

$$\frac{1}{n} - \frac{1}{n+1} = \frac{n+1-n}{n(n+1)} = \frac{1}{n(n+1)} \approx \frac{1}{n^2}.$$

Therefore,

$$r_n = 1 - \frac{1}{n+1} \approx 1 - \frac{1}{n} = r_{n-1},$$

with an error approximately equal to $1/n^2$.

Aitken for the sum

Let $S_n = \sum_{i=0}^{n} c_i$ and assume $\lim_{n \to \infty} S_n = 0$.

This assumption implies $S_{n+1} < S_n$, for sufficiently large n.

And therefore, the ratio r in

$$S_{n+1} - 0 = r\,(S_n - 0) \quad \Rightarrow \quad r = \frac{S_{n+1}}{S_n} < 1.$$

The ratio r depends also on n, but assuming convergence, it is expected that the difference between r_n and r_{n-1} is of a lesser order.

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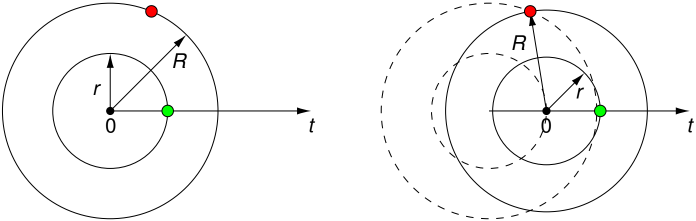
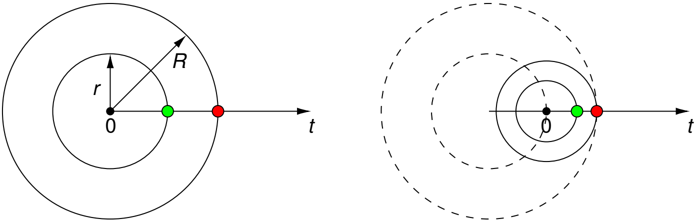
going past versus going towards a singularity

- Going past a singularity (the red dot):



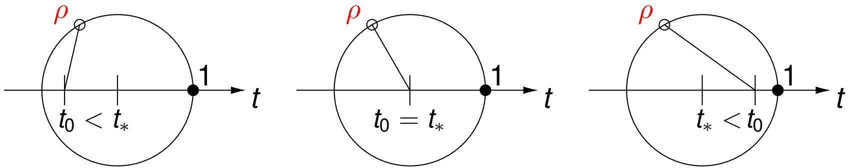
- Going towards a singularity (the red dot):



the last pole

Consider a path $\mathbf{x}(t)$ heading towards $t = 1$.

The *last pole* ρ, marked by the hollow circle on the figure below, is the last value for t, with nonzero imaginary part, for which $\mathbf{x}(t)$ is singular.

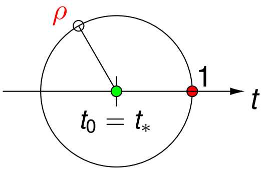


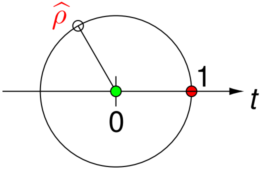
1. $t_0 < t_*$: the proximity to ρ determines the step size.
2. $t_0 = t_*$: the critical equidistant location to ρ and 1.
3. $t_0 > t_*$: we are heading towards the end of the path.

At $t_0 = t_*$, the homotopy will be reconditioned.

recentering and scaling the radius of convergence

At the critical distance to the last pole ρ:





At the right, after recentering the series at $t = 0$ and scaling,
the distance to the closest singularity equals 1,
as in the monomial homotopies case studies.

recenter, scale and shift

At $t_0 = t_*$ is the critical spot between the last pole ρ and 1:

$$R = |\rho - t_*| = |1 - t_*|.$$

The reconditioning of the homotopy involves a scale and shift:

- the scale ensures $R = 1$, then recenter series so $t_* = 0$,
- the shift makes $x(0) = 1$.

Benefits from the reconditioning:

- $R = 1$ avoids excessive growth of decay of the series coefficients.
- $x(0) = 1$ allows the application of $\log(1 - x)$ to detect divergence.

If the shift is omitted, then look at the expansion of $\log(x(0) - x(t))$.

numerical reconditioning of the homotopy

If the radius of convergence of the series $x(t)$ is R,
then, after substitution $t = Rs$, $x(s)$ has convergence radius one.

The reconditioning is limited by the accuracy of the ratio R.

If $R < 1$, then the coefficient growth leads to numerical instabilities.

A staggered and iterative method is needed:

- staggered: for $d = 8, 16, 24, 32, \ldots$, and
- iterative: scale with $R_8, R_{16}, R_{24}, R_{32}, \ldots$.

With extrapolation, R_{64} has an accuracy of 8 decimal places,
but much less accuracy is needed to estimate the magnitude of R.

Multiprecision may be needed for intermediate coefficient growth.

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using partial derivatives

For general singularities, compute a linear combination of the columns of the matrix of all partial derivatives that makes zero.

For example, for $f(x,y) = 0$, $g(x,y) = 0$, consider

$$\left[\begin{array}{cc} \dfrac{\partial f}{\partial x} & \dfrac{\partial f}{\partial y} \\[2ex] \dfrac{\partial g}{\partial x} & \dfrac{\partial g}{\partial y} \end{array} \right] = \left[\begin{array}{cc} a_{1,1}(t) & a_{1,2}(t) \\ a_{2,1}(t) & a_{2,2}(t) \end{array} \right],$$

after substitution of the series $x(t)$ and $y(t)$.

Then apply a QR decomposition to find a nonzero vector that makes a zero vector.

This generalizes the series sums that converge to zero in the monomial homotopy case studies.

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an example of Ojika, 1987

$$\mathbf{f}(x,y) = \left\{ \begin{array}{rcl} x^2 + y - 3 & = & 0 \\ x + 0.125y^2 - 1.5 & = & 0 \end{array} \right.$$

has a triple root at $(1,2)$. Using a total degree start system with random γ, the t_0 after t_* was found at $t_0 = 0.956$.

After reconditioning, with order $n = 64$, the location is estimated at

$$1.0265192231142901 + 2.9197227799819557\mathrm{E}{-}05\, I$$

and improved with Richardson extrapolation to

$$0.9999729580138075 + 8.484367218447337\mathrm{E}{-}06\, I,$$

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

Done with sympy 1.4, mpmath 1.1.0, and phcpy 1.1.1 (CASC 2022).

one fourfold cyclic 9-root

The cyclic 9-roots problem (solved by Faugère in 2001) has several isolated roots of multiplicity four.

With the plain blackbox solver of PHCpack, one path was selected that ended at one of the fourfold roots.

The t_0 after t_*, the location of the last pole, is $t_0 = 0.99832$.

After reconditioning, with $n = 32$, the convergence radius is

$$1.00000000099639 + 4.319265\text{E}{-}09\, I$$

and confirmed in double double precision.

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

conclusions

Assuming effective methods (symbolic, Newton, Fourier, ...) to compute Taylor series, singularities can be located and approximated.

Taylor series are a better tool than the singular value decomposition, because with Taylor series we are at a safe distance from singularities.

- Reconditioning the homotopy is needed for numerical stability.
- Use $\log(x(0) - x(t))$ to decide if $x(t)$ converges or not.
- Richardson extrapolation is effective for the convergence radius. Aitken extrapolation works too.
- To compute the coordinates of singular solutions, Aitken extrapolation is sensitive to the winding numbers.