Extrapolating on Taylor Series Solutions of Homotopies with Nearby Poles

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Extrapolating on Taylor Series Solutions

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polynomial homotopy continuation

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

For example, the homotopy

$$h(\mathbf{x}, t) = (1 - t)g(\mathbf{x}) + t\, f(\mathbf{x}) = \mathbf{0}$$

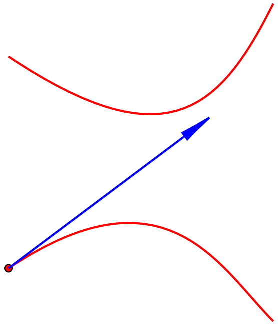
connects

- the target system $f(\mathbf{x}) = \mathbf{0}$, at $t = 1$, to the
- the start system $g(\mathbf{x}) = \mathbf{0}$, at $t = 0$.

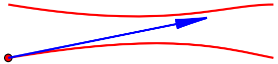
Continuation methods apply path tracking algorithms to track solution paths $x(t)$ starting at solutions of $g(\mathbf{x}) = \mathbf{0}$ and ending at the solutions of $f(\mathbf{x}) = \mathbf{0}$.

the path jumping problem

Curves are far apart, with high curvature:



Curves are close to each other, with low curvature:



a priori step size control

- 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.
- S. Telen, M. Van Barel, and J. Verschelde.
Robust Numerical Tracking of One Path of a Polynomial Homotopy on Parallel Shared Memory Computers.
In the *Proceedings of the 22nd International Workshop on Computer Algebra in Scientific Computing (CASC 2020)*, pages 563–582. Springer-Verlag, 2020.

Main results:

1. a new *a priori step size control* algorithm,
2. runs in practice on homotopies of millions of paths,
3. error analysis on the growth of Taylor series coefficients.

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* $\lim_{n \rightarrow \infty} c_n / c_{n+1} = z$, *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 $|z|$.

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

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

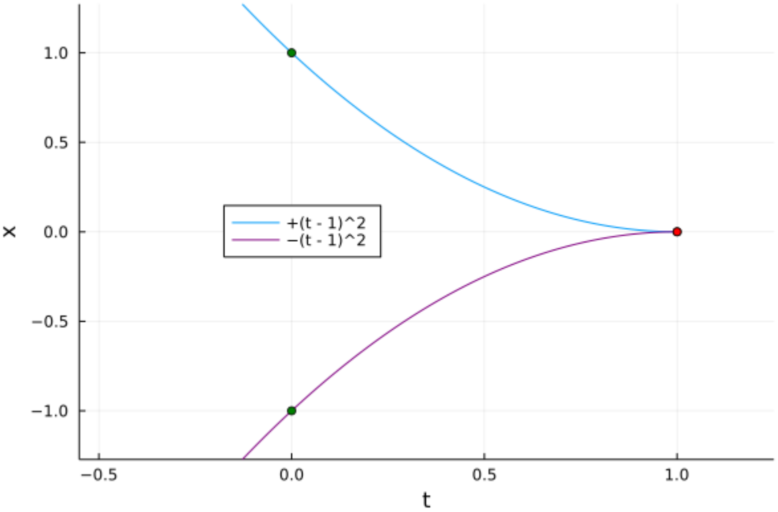
$$\begin{array}{rcl}(c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4)(1 + b_1 t) & = & a_0 + a_1 t + a_2 t^2 + a_3 t^3 \\ c_0 + \quad c_1 t + \quad c_2 t^2 + \quad c_3 t^3 + \quad c_4 t^4 & & \\ + b_1 c_0 t + b_1 c_1 t^2 + b_1 c_2 t^3 + b_1 c_3 t^4 & = & a_0 + a_1 t + a_2 t^2 + a_3 t^3\end{array}$$

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

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



problem statement

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.

How many terms in the Taylor series are needed to solve the location problem?

Our prior work:
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.

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Taylor series of roots of a polynomial homotopy

Consider the monomial homotopy

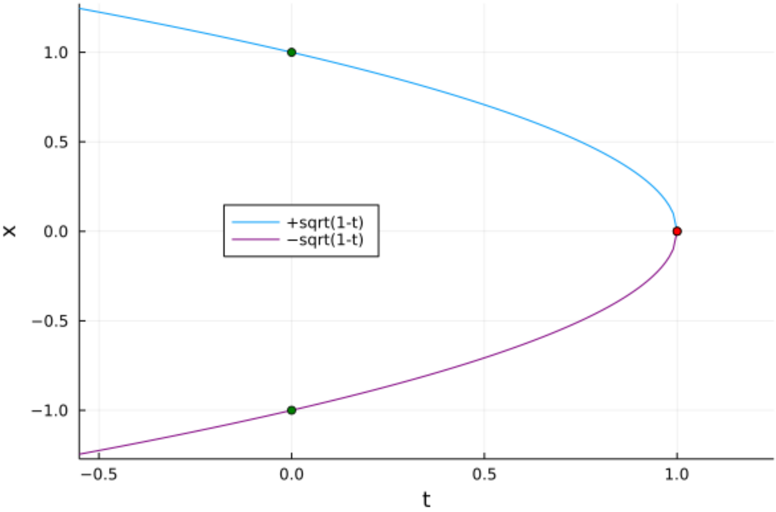
$$h(x, t) = x^2 - 1 + t = 0,$$

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.

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



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

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

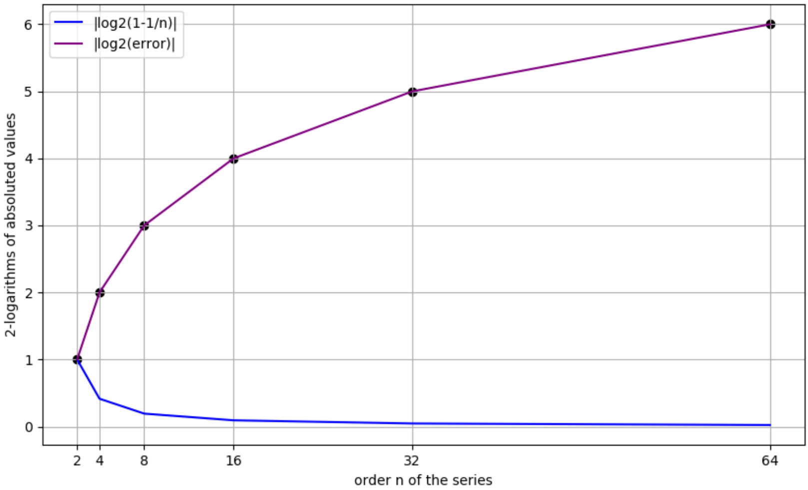
for sufficiently large n.

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*



the Rho Algorithm

Let c_n be the nth coefficient of the Taylor series of $x(t) = \sqrt{1 - t}$.

Then $f(n) = \dfrac{c_n}{c_{n+1}} = \dfrac{2(n+1)}{2n-1}$.

$f(k)$ converges logarithmically to 1, $f(64)$ has an error of `1.2e-02`.

- Richardson extrapolation gives an error of `3.8e-08`,
- improved by repeated Aitken to an error of `2.3e-11`.

The Rho Algorithm (Wynn, 1955) needs 4 terms for a correct result.

The Rho Algorithm computes even order convergents of Thiele's interpolating continued fraction.
Thiele interpolation recovers $f(n)$ with just 4 points.

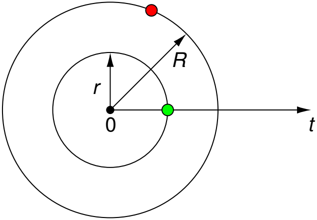
the Rho algorithm in Python

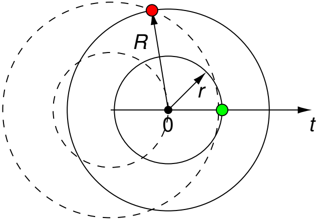
```
def rhoComplex(nbr):
    """
    Runs the rho algorithm in complex double arithmetic,
    on the numbers given in the list nbr, using x(n) = n+1.
    Returns the last element of the table
    of extrapolated numbers.
    """
    rho1 = [1.0/(nbr[n] - nbr[n-1])
            for n in range(1, len(nbr))]
    rho = [nbr, rho1]
    for k in range(2, len(nbr)):
        nextrho = []
        for n in range(k, len(nbr)):
            invrho1 = complex(k)/
                (rho[k-1][n-k+1] - rho[k-1][n-k])
            nextrho.append(rho[k-2][n-k+1] + invrho1)
        rho.append(nextrho)
    return nextrho[-1]
```

Used in *Extrapolating Solution Paths of Polynomial Homotopies towards Singularities with PHCpack and phcpy*, ICMS 2024.

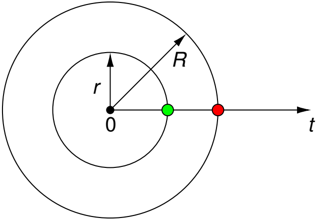
going past versus going towards a singularity

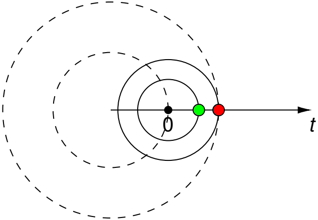
- Going past a singularity (the red dot):





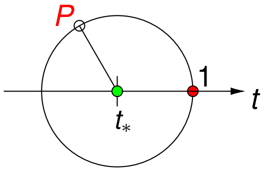
- Going towards a singularity (the red dot):





recentering and scaling the radius of convergence

At the critical distance to the last pole P:



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.

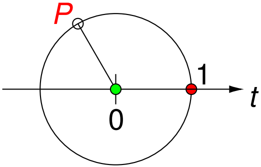
Definition (the last pole)

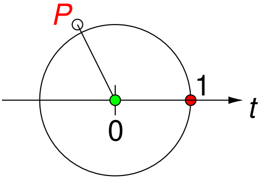
Given a solution path $\mathbf{x}(t)$ of a homotopy $h(\mathbf{x}, t) = \mathbf{0}$, *the last pole* P is a value for t such that

1. the matrix of all partial derivatives of $h(\mathbf{x}(P), P)$ is rank deficient,
2. of all poles, $\mathrm{re}(P)$ is closest to the left of 1.

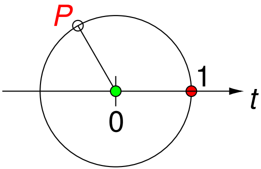
Past the Critical Distance

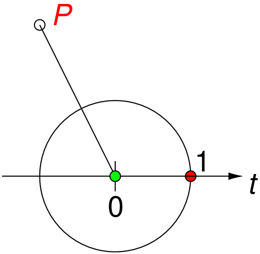
Just past the critical distance, the last pole P is at $-\frac{1}{2} + I$:





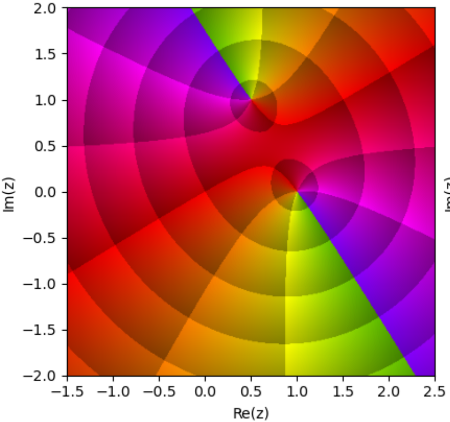
More past the critical distance, the last pole P is at $-1 + 2I$:

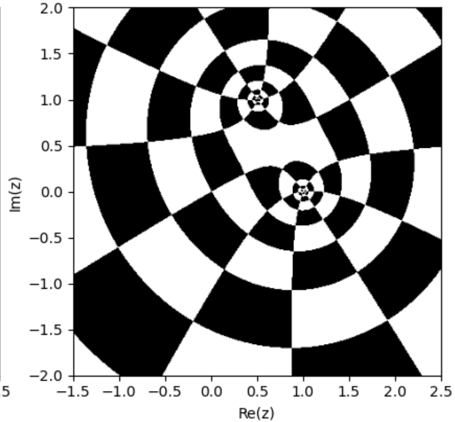




a phase portrait

$f(z) = \sqrt{4/5(1/2 - I)(1 - z)(1/2 + I - z)}$, phase $f/|f|$ is at left:





At the right is a polar chessboard.

Used `complexplorer-0.1.2` of I. Kuvychko, with `matplotlib`.

running the Rho Algorithm

The Rho Algorithm is applied on the sequence c_n/c_{n+1}, $k = 0, 1, \ldots d$,

- c_n is the nth coefficient of the Taylor series of $x(t)$, and
- $x(t) = \sqrt{a(1-t)(P-t)}$, where a is such that $x(0) = 1$.

The smallest error of the rho table for various P and d values:

P	$d = 8$	$d = 16$	$d = 32$
$-1/2 + I$	5.0e-01	3.5e-01	1.4e-01
$-1/2 + 2I$	1.7e-01	9.8e-03	2.6e-05
$-1 + 4I$	2.5e-02	6.9e-05	6.3e-09
$-2 + 8I$	3.3e-03	5.3e-07	3.5e-11
$-4 + 16I$	4.1e-04	4.0e-09	2.4e-12

All calculations happened in double precision.
The coefficients c_n were computed with tolerance `1.0e-12`.

Extrapolating on Taylor Series Solutions

a motivating lemma

Lemma (a motivating lemma)

Let a_n by the n-th coefficient of the Taylor series $x(t)$ defined by

$$x^q = (1-t)^p, \quad t \in [0,1], \quad p \geq 1, \quad q \geq 2.$$

Then:

$$\frac{a_n}{a_{n+1}} = 1 + \sum_{k=1}^{\infty} \alpha_k \left(\frac{1}{n} \right)^k,$$

for coefficients α_k independent of n.

Because of this error expansion in $(1/n)$, extrapolation works.

two nearby poles

Lemma (two nearby poles)

Let $\mathbf{a} = (a_k)_{k=0}^{\infty}$ *and* $\mathbf{b} = (b_k)_{k=0}^{\infty}$ *be sequences of nonzero numbers. Assume the convolution* $\mathbf{c} = \mathbf{a} \star \mathbf{b}$ *yields another sequence of nonzero numbers* $\mathbf{c} = (c_k)_{k=0}^{\infty}$*. Then we have*

$$\frac{c_n}{c_{n+1}} = \left(\frac{a_n}{a_{n+1}} \right) \sum_{k=0}^{n} \frac{1}{\displaystyle \sum_{\ell=0}^{n+1} \left(\frac{a_n}{a_{n+1}} \right) \left(\frac{a_\ell}{a_k} \right) \left(\frac{b_{n+1-\ell}}{b_{n-k}} \right)}.$$

Unlike the motivating Lemma,
there is no error expansion suitable for extrapolation to work.

a far away pole

Lemma (a far away pole)

For P such that $|P| \gg 1$, for indices $k > 0$ and $\ell > 0$, and for nonzero coefficients $a_k, a_{k-1}, \ldots, a_{-\ell+1}, a_{-\ell}$, consider

$$Q = \frac{1}{a_k P^k + a_{k-1} P^{k-1} + \cdots + a_{-\ell+1} P^{-\ell+1} + a_{-\ell} P^{-\ell}.}$$

Coefficients β_i exist so Q can be written as

$$Q = \sum_{i=k}^{\infty} \beta_i \left(\frac{1}{P} \right)^i .$$

Theorem (conditions for extrapolation to work)

Consider two series $x(t)$ and $y(t)$, each with a unique nearby singularity, 1 and P, respectively,

$$x(t) = \sum_{k=0}^{\infty} a_k t^k, \quad \lim_{n \to \infty} \frac{a_n}{a_{n+1}} = 1,$$

and

$$y(t) = \sum_{k=0}^{\infty} b_k t^k, \quad \lim_{n \to \infty} \frac{b_n}{b_{n+1}} = P, \quad |P| \gg 1.$$

Let $z(t) = x(t) \star y(t)$, with $z(t) = \sum_{k=0}^{\infty} c_k t^k$. Then, for sufficiently large N and M, $M > N$, we have for all $n \geq N$ and $n \leq M$:

$$\frac{c_n}{c_{n+1}} = 1 + \sum_{k=1}^{\infty} \gamma_k \left(\frac{1}{n} \right)^k,$$

for constants γ_k computed for n in $[N, M]$.

conclusions

We provide a condition for the effectiveness of extrapolation methods to accelerate slowly converging Taylor series of solution paths of polynomial homotopies, extending our results of CASC 2022.

The main application is in the accurate approximation of isolated singular solutions at the end of solution paths.

For the proofs, see `arXiv:2404.17681 [math.NA]`.