Robust Numerical Path Tracking for Polynomial Homotopies

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joint work with Simon Telen and Marc Van Barel

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Outline

1. Problem Statement
   - adaptive step control
   - Padé approximants and power series

2. Detecting Nearby Singularities
   - applying the ratio theorem of Fabry
   - an illustrative example

3. Distance to the Nearest Path
   - an estimate based on the Jacobian and Hessian matrices
   - an illustrative example

4. Algorithm and Computational Experiments
   - an apriori step control algorithm
   - two generic polynomials
   - the 184,756 paths to all cyclic 11-roots
Robust Numerical Path Tracking

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problem statement

To solve a polynomial system $f(x) = 0$, the homotopy

$$h(x, t) = \gamma(1 - t)g(x) + tf(x) = 0,$$

defines solution paths $x(t)$ satisfying $h(x(t), t) = 0$, where

- $\gamma \in \mathbb{C}$ is a random constant,
- $t \in [0, 1]$ is the continuation parameter,
- $g(x) = 0$ is the start system, with known solutions $x(0)$,
- $f(x) = 0$ is the target system, with solutions $x(1)$.

If all solutions of $g(x) = 0$ are regular, then, except for a finite number of bad choices of $\gamma$, all solution paths $x(t)$ are regular, for all $t < 1$.

Variable step size $\Delta t$ control in predictor-corrector methods:

- $\Delta t$ is too large: divergence and/or path jumping.
- $\Delta t$ is too small: inefficient, we care only about $x(1)$. 
five relevant papers, in chronological order


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Padé Approximants

Consider the homotopy: 

\[(1 - t)(x^2 - 1) + t(3x^2 - 3/2) = 0.\]

a posteriori and a priori step control

An *a posteriori* step control uses feedback loops.

\[ \Delta t := \beta \Delta t \]

**predictor** → **corrector**

\[ \| \mathbf{f}(\mathbf{z}(\Delta t)) \| > \alpha \]

\[ \| \mathbf{f}(\mathbf{z}(\Delta t)) \| > \epsilon \]

Extreme choices for $\alpha$ and $\epsilon$ (not recommended):
- If $\alpha \leq \epsilon$, then the corrector is not needed.
- If $\alpha = \infty$, then the first feedback loop does never happen.

Setting 0.5 for $\beta$ cuts the step size $\Delta$ in half.

Our goal: develop an *a priori* step control algorithm.
linearization

Working with truncated power series, computing modulo $O(t^d)$, is doing arithmetic over the field of formal series $\mathbb{C}[[t]]$.

Linearization: consider $\mathbb{C}^n[[t]]$ instead of $\mathbb{C}[[t]]^n$. Instead of a vector of power series, we consider a power series with vectors as coefficients.

Solve $Ax = b$, $A \in \mathbb{C}^{n \times n}[[t]]$, $b, x \in \mathbb{C}^n[[t]]$.

\begin{align*}
A &= A_0 t^a + A_1 t^{a+1} + \cdots, \\
b &= b_0 t^b + b_1 t^{b+1} + \cdots \\
x &= x_0 t^{b-a} + x_1 t^{b-a+1} + \cdots \\
\end{align*}

where $A_i \in \mathbb{C}^{n \times n}$ and $b_i, x_i \in \mathbb{C}^n$. 
Computing the first \( d \) terms of the solution of \( Ax = b \):

\[
(A_0 t^a + A_1 t^{a+1} + A_2 t^{a+2} + \ldots + A_d t^{a+d}) \cdot (x_0 t^{b-a} + x_1 t^{b-a+1} + x_2 t^{b-a+2} + \ldots + x_d t^{b-a+d}) = b_0 t^b + b_1 t^{b+1} + b_2 t^{b+2} + \ldots + b_d t^{b+d}.
\]

Written in matrix format:

\[
\begin{bmatrix}
A_0 & A_1 & A_0 \\
A_1 & A_0 & A_0 \\
A_2 & A_1 & A_0 \\
\vdots & \vdots & \vdots \\
A_d & A_{d-1} & A_{d-2} & \ldots & A_0
\end{bmatrix}
\begin{bmatrix}
x_0 \\
x_1 \\
x_2 \\
\vdots \\
x_d
\end{bmatrix}
=
\begin{bmatrix}
b_0 \\
b_1 \\
b_2 \\
\vdots \\
b_d
\end{bmatrix}.
\]

If \( A_0 \) is regular, then solving \( Ax = b \) is straightforward.
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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 \( \lim_{n \to \infty} \frac{c_n}{c_{n+1}} = z \), 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 \(|z|\).

L. Leau in 1899 comments on the proof (Bieberbach, 1955, page 51): “d’habiles calculs malheureusement assez complexes.”

the ratio theorem of Fabry and Padé approximants

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

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

\[
(c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4)(1 + b_1 t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3
\]

\[
c_0 + c_1 t + c_2 t^2 + c_3 t^3 + c_4 t^4 + b_1 c_0 t + b_1 c_1 t^2 + b_1 c_2 t^3 + b_1 c_3 t^4 = a_0 + a_1 t + a_2 t^2 + a_3 t^3
\]

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 \([3/1]_x\) is \( 1 - c_4 / c_3 t \). The pole of \([3/1]_x\) is \( c_3 / c_4 \).
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   - an illustrative example

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an illustrative example

Consider the homotopy $x^2 - (t - 1/2)^2 - p^2 = 0$, for $p > 0$.

$$x(t) = \pm \sqrt{4p^2 + 4t^2 - 4t + 1}$$

two nearby singularities for complex values of $t$

$$4p^2 + 4t^2 - 4t + 1 = 0 \Rightarrow t = \frac{1}{2} \pm p\sqrt{-1}$$
poles of a [6/2]-Padé approximant

\[ x(t) = \sqrt{4p^2 + 4t^2 - 4t + 1} \] for \( p = 0.1 \)

has singularities at \( t = 0.5 \pm 0.1I \).

<table>
<thead>
<tr>
<th>( t )</th>
<th>poles</th>
<th>radius</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.522 ± 0.054I</td>
<td>0.525</td>
</tr>
<tr>
<td>0.1</td>
<td>0.428 ± 0.056I</td>
<td>0.431</td>
</tr>
<tr>
<td>0.2</td>
<td>0.336 ± 0.061I</td>
<td>0.341</td>
</tr>
<tr>
<td>0.3</td>
<td>0.250 ± 0.077I</td>
<td>0.261</td>
</tr>
<tr>
<td>0.4</td>
<td>0.139 ± 0.126I</td>
<td>0.188</td>
</tr>
<tr>
<td>0.5</td>
<td>±0.126I</td>
<td>0.126</td>
</tr>
</tbody>
</table>

The poles of the Padé approximant predict the distance to the nearest singularity.
approaching a nearby singularity – step 0

The circle centered at $t = 0.0$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
approaching a nearby singularity – step 1

The circle centered at $t = 0.1$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1I$ are represented by the red dots.
approaching a nearby singularity – step 2

The circle centered at $t = 0.2$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
approaching a nearby singularity – step 3

The circle centered at $t = 0.3$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
approaching a nearby singularity – step 4

The circle centered at $t = 0.4$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1I$ are represented by the red dots.
close to a nearby singularity – step 5

The circle centered at $t = 0.5$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
leaving a nearby singularity – step 6

The circle centered at $t = 0.6$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1/|I|$ are represented by the red dots.
leaving a nearby singularity – step 7

The circle centered at $t = 0.7$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
leaving a nearby singularity – step 8

The circle centered at $t = 0.8$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
leaving a nearby singularity – step 9

The circle centered at $t = 0.9$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
leaving a nearby singularity – step 10

The circle centered at $t = 1.0$ has as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1I$ are represented by the red dots.
approaching and leaving a nearby singularity

Circles centered at $t = 0.0, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$ have as radius the computed distance to the closest pole.

The singular points at $0.5 \pm 0.1i$ are represented by the red dots.
a phcpy session with a [6/2]-Padé predictor
phcpy is the Python interface to PHCpack

\[
t : 4.93828714960806E-01 \quad 0.00000000000000E+00
\]
\[
m : 1
\]

the solution for t :

\[
x : 1.00190242833497E-01 \quad 0.00000000000000E+00
\]
\[
== err : 4.795E-09 = rco : 1.000E+00 = res : 1.210E-17 =
\]

\[
t : 4.938e-01, \ step : 9.383e-02, \ frp : 1.877e-01
\]

closest pole : (0.13875598086124408, -0.1263411602765256)

poles: 

\[
[(0.13875598086124408-0.1263411602765256j),
(0.1387559808612441+0.1263411602765256j)]
\]

- The poles are computed at \( t = 0.4 \).
- The tracker slows down before 0.5.
- The imaginary parts of the poles are close in magnitude to \( 0.1 = \rho \).
the approximation error of the Padé approximant

Consider the Padé approximant \([L/M]_k = p_k(t)/q_k(t)\), with degrees \(\text{deg}(p_k) = L\), \(\text{deg}(q_k) = M\), \(k = 1, 2, \ldots, n\), for the \(k\)th coordinate \(x_k(t)\) of the solution around \(t = 0\).

For small step size \(\Delta t\), we estimate the error, for \(\ell = L + M + 2\),

\[
e_k(\Delta t) = \frac{p_k(\Delta t)}{q_k(\Delta t)} - x_k(\Delta t) = e_{0,k}(\Delta t)^\ell + O((\Delta t)^{\ell+1}).
\]

Using \(|e_k(\Delta t)| \approx |e_{0,k}(\Delta t)^\ell|\) leads to

\[
\left\|x(\Delta t) - \left(\frac{p_1(\Delta t)}{q_1(\Delta t)}, \frac{p_2(\Delta t)}{q_2(\Delta t)}, \ldots, \frac{p_n(\Delta t)}{q_n(\Delta t)}\right)\right\| \approx \|e_0\| |\Delta t|^{\ell},
\]

with \(e_0 = (e_{0,1}, e_{0,2}, \ldots, e_{0,n})\).
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distance to the nearest path

Let $y(t)$ and $z(t)$ be two distinct solution paths of $h(x, t) = 0$. We assume $z(t)$ is close to $y(t)$ and denote $\Delta z = y(t) - z(t) \in \mathbb{C}^n$. Our goal is to estimate $\|\Delta z\|$.

$$h(y(t), t) \approx h(z(t), t) + J_h(z(t), t)\Delta z + \frac{\nu}{2},$$

where $J_h$ is the Jacobian matrix,

$$\nu = \begin{bmatrix}
\langle \mathcal{H}_1(z(t), t)\Delta z, \Delta z \rangle \\
\langle \mathcal{H}_2(z(t), t)\Delta z, \Delta z \rangle \\
\vdots \\
\langle \mathcal{H}_n(z(t), t)\Delta z, \Delta z \rangle 
\end{bmatrix}$$

$\mathcal{H}_k(x, t) = \frac{\partial^2 h_k}{\partial x_\ell \partial x_m}$, $1 \leq \ell, m \leq n$.

$\mathcal{H}_k$ is the Hessian of the homotopy $h_k$, and $\langle \cdot, \cdot \rangle$ is the inner product.
the largest singular values of the Hessians

Abbreviate $J_h(z(t), t)$ by $J_h$ and $\mathcal{H}_k(z(t), t)$ by $\mathcal{H}_k$:

$$0 \approx 0 + J_h \Delta z + \frac{1}{2} \begin{bmatrix} 
\langle \mathcal{H}_1 \Delta z, \Delta z \rangle \\
\langle \mathcal{H}_2 \Delta z, \Delta z \rangle \\
\vdots \\
\langle \mathcal{H}_n \Delta z, \Delta z \rangle 
\end{bmatrix}.$$

The Hessian matrices are Hermitian and have a unitary diagonalization $\mathcal{H}_k = V_k \Lambda_k V_k^H$, for the Hermitian transpose $\cdot^H$, $V_k^H V_k = I$.

There is some vector $w_k$ such that $\|w_k\| = \|\Delta z\|$ and $\Delta z = V_k w_k$.

$$\langle \mathcal{H}_k \Delta z, \Delta z \rangle = \langle \Lambda_k w_k, w_k \rangle$$

$$\Rightarrow \ |\langle \mathcal{H}_k \Delta z, \Delta z \rangle| \leq \sigma_{k,1} \|w_k\|^2 = \sigma_{k,1} \|\Delta z\|^2,$$

for the largest singular value $\sigma_{k,1}$ of $\mathcal{H}_k$. 
the smallest singular value of the Jacobian matrix

Applying $|\langle H_k \Delta z, \Delta z \rangle| \leq \sigma_{k,1} \|\Delta z\|^2$ leads to

$$\begin{bmatrix} \langle H_1 \Delta z, \Delta z \rangle \\ \langle H_2 \Delta z, \Delta z \rangle \\ \vdots \\ \langle H_n \Delta z, \Delta z \rangle \end{bmatrix} \leq \begin{bmatrix} \sigma_{1,1} \|\Delta z\|^2 \\ \sigma_{2,1} \|\Delta z\|^2 \\ \vdots \\ \sigma_{n,1} \|\Delta z\|^2 \end{bmatrix} = \|\Delta z\|^2 \sqrt{\sigma_{1,1}^2 + \sigma_{2,1}^2 + \cdots + \sigma_{n,1}^2}.$$

As we have an upper bound for the right hand side of

$$J_h \Delta z \approx -\frac{1}{2} \begin{bmatrix} \langle H_1 \Delta z, \Delta z \rangle \\ \langle H_2 \Delta z, \Delta z \rangle \\ \vdots \\ \langle H_n \Delta z, \Delta z \rangle \end{bmatrix}$$

we use a lower bound for the left hand side: $\|J_h \Delta z\| \geq \sigma_n(J_h) \|\Delta z\|$, where $\sigma_n(J_h)$ is the smallest singular value of the Jacobian matrix $J_h$. 
an estimate for the distance to the nearest path

\[
\sigma_n(J_h) \| \Delta z \| \leq \| J_h \Delta z \| \approx \frac{1}{2} \left\| \begin{array}{c} \langle \mathcal{H}_1 \Delta z, \Delta z \rangle \\ \langle \mathcal{H}_2 \Delta z, \Delta z \rangle \\ \vdots \\ \langle \mathcal{H}_n \Delta z, \Delta z \rangle \end{array} \right\| \\
\leq \frac{1}{2} \| \Delta z \|^2 \sqrt{\sigma_{1,1}^2 + \sigma_{2,1}^2 + \cdots + \sigma_{n,1}^2} \\
\Downarrow \\
\frac{2\sigma_n(J_h)}{\sqrt{\sigma_{1,1}^2 + \sigma_{2,1}^2 + \cdots + \sigma_{n,1}^2}} \lesssim \| \Delta z \| 
\]

The lower bound for \( \| \Delta z \| \) decreases

- as \( J_h \) becomes close to a singular matrix, and/or
- as the curvature of the path increases.
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   - an illustrative example

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Consider the homotopy \( h(x, t) = x^{p+1} - q(x - (t - 1/2)) = 0 \), where

- \( p \in \mathbb{Z}^+ \) controls the curvature.
- \( q \in \mathbb{R}^+ \) controls the distance to the nearest solution.

At \( t = 1/2 \): \( h(x, t = 1/2) = (x^p - q)x = 0 \). Consider \( z = q^{1/p} \).

- \( J_h = (p + 1)x^p - q \), \( J_h(x = z) = (p + 1)q - q = pq \),
  for fixed \( p \), small \( q \), the Jacobian \( J_h \) is close to singular.
- \( \mathcal{H} = (p + 1)px^{p-1} \), \( \mathcal{H}(x = z) = (p + 1)pq^{(p-1)/p} \),
  for fixed \( q \), the Hessian \( \mathcal{H} \) grows quadratically in \( p \).

\[
|\Delta z| \geq \frac{J_h(x = z)}{\mathcal{H}(x = z)} = \frac{q}{(p + 1)q^{(p-1)/p}}
\]

\( z = q^{1/p} \): small \( q \ll 1 \): the lower bound for \( |\Delta z| \) decreases for all \( p \),
large \( q \gg 1 \): the lower bound for \( |\Delta z| \) decreases for large \( p \).
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   - an illustrative example

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To determine the step size $\Delta t$, do as follows:

1. Compute the distance $R$ to the closest pole.

2. Compute the lower bound $L = \frac{2\sigma_n(J_h)}{\sqrt{\sigma_{1,1}^2 + \sigma_{2,1}^2 + \cdots + \sigma_{n,1}^2}}$ on the distance to the nearest path.

3. Use the approximation error of the Padé approximant:

   $$\left\| \frac{p_1(\Delta t)}{q_1(\Delta t)} - \frac{p_2(\Delta t)}{q_2(\Delta t)} - \cdots - \frac{p_n(\Delta t)}{q_n(\Delta t)} \right\| \approx \| e_0 \| |\Delta t|^\ell,$$

   compute $\| e_0 \| |\Delta t|^\ell \leq L \Rightarrow \Delta t \leq \left( \frac{L}{\| e_0 \|} \right)^{1/\ell} = D$.

4. $\Delta t = \min(\beta_1 R, \beta_2 D)$, for some constants $\beta_1, \beta_2$, $0 < \beta_1, \beta_2 < 1$. 

Jan Verschelde (UIC)
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two generic polynomials

Two polynomials of degree \(d\) lead to a homotopy with \(d^2\) paths.

```
phc -p: a posteriori step control with corrector feedback loop
phc -u: a priori step control based on poles and Hessians
```

<table>
<thead>
<tr>
<th>(d)</th>
<th>(d^2)</th>
<th>#fail</th>
<th>user cpu time</th>
<th>#fail</th>
<th>user cpu time</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>100</td>
<td>0</td>
<td>124ms</td>
<td>0</td>
<td>5s 130ms</td>
</tr>
<tr>
<td>20</td>
<td>400</td>
<td>2</td>
<td>2s 59ms</td>
<td>0</td>
<td>1m 11s 610ms</td>
</tr>
<tr>
<td>30</td>
<td>900</td>
<td>8</td>
<td>10s 462ms</td>
<td>0</td>
<td>6m 10s 521ms</td>
</tr>
<tr>
<td>40</td>
<td>1600</td>
<td>23</td>
<td>33s 558ms</td>
<td>0</td>
<td>20m 19s 950ms</td>
</tr>
<tr>
<td>50</td>
<td>2500</td>
<td>39</td>
<td>1m 13s 489ms</td>
<td>0</td>
<td>44m 0s 807ms</td>
</tr>
</tbody>
</table>

Ran on one core of 3.1 GHz Intel Core i7, 16 GB 1867 MHz DDR3, in double precision, early 2015 MacBook Pro, macOS Sierra 10.12.6.

Done with version 2.4.67, `phc -u` is still under development.
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The cyclic 11-roots problem is a sparse polynomial system
- in 11 variables with 181,756 isolated solutions;
- the mixed volume of the Newton polytopes equals 181,756.

The start system is a system with the same Newton polytopes, but with randomly generated complex coefficients.

A run with `phc` on some difficult path shows:
- Around $t = 0.5$, the coordinates take extreme values, suggesting a diverging path.
- But there is no nearby pole at $t = 0.5$ and `phc -u` can complete without the bound involving the Jacobian and Hessians.

These computations are confirmed with the program `Padé.jl`, Julia code written by Simon Telen and Marc Van Barel.

*work still in progress...*