Polynomial Continuation for Singular Solutions

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Outline

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   - reconditioning singularities with deflation
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   - detection and location of quadratic turning points

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   - Puiseux series and the determinant criterion

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Solving Polynomial Systems

numerical algebraic geometry: numerical analysis and algebraic geometry

Polynomial systems are nonlinear systems with algebraic structure.
This algebraic structure enables to compute

- not only **all** isolated solutions,
- but also **a numerical irreducible decomposition**
  $\longrightarrow$ degrees and dimensions of all irreducible components.

Two key references:

1. **Tien-Yien Li.** Numerical solution of polynomial systems by homotopy continuation methods. In Volume XI of *Handbook of Numerical Analysis*, pages 209–304, 2003.
2. **Andrew J. Sommese and Charles W. Wampler.** *The Numerical Solution of Systems of Polynomials Arising in Engineering and Science.* World Scientific, 2005.

Homotopy Continuation Methods

natural and artificial parameter homotopies

A **homotopy** h is a family of systems, depending on a parameter.
With **continuation** methods we track solution paths defined by h.
We distinguish between two types of parameters:

1. a natural parameter λ, for example:

$$h(\lambda, x) = \lambda^2 + x^2 - 1 = 0.$$

   As λ varies we track the unit circle: $(\lambda, x(\lambda)) \in h^{-1}(0)$.

2. an artificial parameter t, for example:

$$h(t, \lambda, x) = \left\{ \begin{array}{r} \lambda^2 + x^2 - 1 = 0 \\ (\lambda - 2)t + (\lambda + 2)(1 - t) = 0. \end{array} \right.$$

   As t moves from 0 to 1, λ goes from -2 to $+2$
   and we ***sweep*** points $(\lambda(t), x(\lambda(t)))$ on the unit circle.

Reconditioning Singularities via Deflation

restoring the quadratic convergence of Newton's method

A solution $\mathbf{z}$ to $f(\mathbf{x}) = \mathbf{0}$, $f = (f_1, f_2, \ldots, f_N)$, $\mathbf{x} = (x_1, x_2, \ldots, x_n)$, $N > n$, is **singular** if the Jacobian matrix $A(\mathbf{x}) = \left[\frac{\partial f_i}{\partial x_j} \right]$ has rank $R < n$ at $\mathbf{z}$.

Choose $\mathbf{c} \in \mathbb{C}^{R+1}$ and $\mathbf{B} \in \mathbb{C}^{n \times (R+1)}$ at random.
Introduce $R + 1$ new multiplier variables $\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_{R+1})$.
Apply the Gauss-Newton method to

$$\left\{ \begin{array}{rcl} f(\mathbf{x}) & = & \mathbf{0} \\ A(\mathbf{x})\mathbf{B}\boldsymbol{\mu} & = & \mathbf{0} \\ \mathbf{c}\boldsymbol{\mu} & = & 1 \end{array} \right. \qquad \begin{array}{c} \mathrm{Rank}(A(\mathbf{x})) = R \\ \Downarrow \\ \mathrm{coRank}(A(\mathbf{x})\mathbf{B}) = 1 \end{array}$$

Recurse if necessary, $\#$*deflations* $<$ multiplicity.
An efficient implementation uses algorithmic differentiation.

Problems and Applications

some hard motiviating questions

General problem statement:

Given a polynomial system $f(\boldsymbol{\lambda}, \mathbf{x}) = 0$, $\boldsymbol{\lambda} \in \mathbb{C}^m$, $\mathbf{x} \in \mathbb{C}^n$, find values $\boldsymbol{\lambda}$ for which solutions $\mathbf{x}$ are singular.

Two motivating questions:

- from real algebraic geometry:
  $\rightarrow$ *can all complex solutions turn* **real***?*
- from numerical algebraic geometry:
  $\rightarrow$ *what are the* **real** *irreducible solution components?*

Complexity Issues

of local and global solutions

Solving the global problem

> Given a polynomial system $f(\boldsymbol{\lambda}, \mathbf{x}) = 0$, $\boldsymbol{\lambda} \in \mathbb{C}^m$, $\mathbf{x} \in \mathbb{C}^n$,
> find values $\boldsymbol{\lambda}$ for which solutions $\mathbf{x}$ are singular.

involves a description of **the discriminant variety**
and the solution of more difficult polynomial systems.

Instead we consider a **local** problem, for *one* parameter λ:

Given	a polynomial system $f(\lambda, \mathbf{x}) = 0$, $\boldsymbol{\lambda} \in \mathbb{C}^m$, $\mathbf{x} \in \mathbb{C}^n$,
	a solution $\mathbf{z}$ for $\lambda = \lambda_0$ and target value λ_1,
find	either the solution $\mathbf{z}$ for $\lambda = \lambda_1$
	if no singularities for all $\lambda(t) = (1-t)\lambda_0 + t\lambda_1$,
	or the first $(t, \lambda(t), \mathbf{x}(t))$ for which $\mathbf{z} = (\lambda(t), \mathbf{x}(t))$ is singular.

References

numerical methods

1. **W.J.F. Govaerts.** *Numerical Methods for Bifurcations of Dynamical Equilibria*. SIAM, 2000.
2. **Z. Mei.** *Numerical Bifurcation Analysis for Reaction-Diffusion Equations*. Springer, 2000.
3. **P. Kunkel.** A tree-based analysis of a family of augmented systems for the computation of singular points. *IMA J. Numer. Anal.* 1996.
4. **T.Y. Li and Z. Zeng.** Homotopy continuation algorithm for the real nonsymmetric eigenproblem: Further development and implementation. *SIAM J. Sci. Comput.* 1999.
5. **A. Leykin, J. Verschelde, and A. Zhao.** Newton's method with deflation for isolated singularities of polynomial systems. *Theoretical CS* 2006.
6. **Y. Lu, D.J. Bates, A.J. Sommese, and C.W. Wampler.** Finding all real points of a complex curve. To appear in *Contemporary Mathematics*.

Quadratic Turning Points

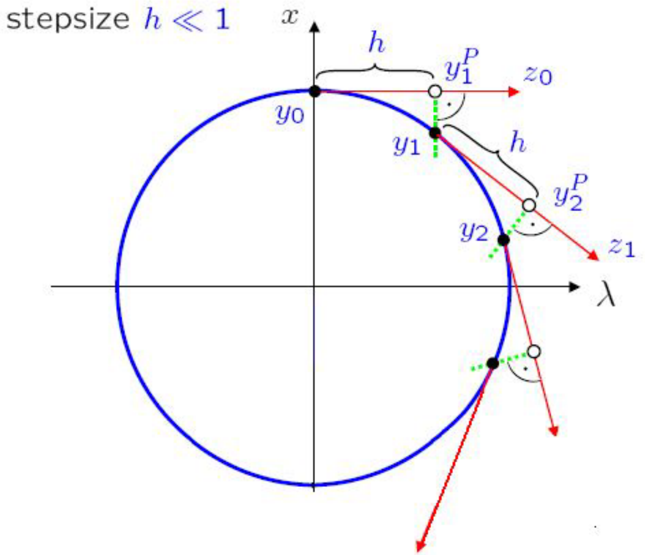
most common type of singularity

1. **Definition:** solution paths turn back
   when the parameter increases past a quadratic turning point.
   Properties: a double solution, corank of Jacobian equals one,
   transition point: complex $\leftrightarrow$ real.

2. **Detection:** monitor orientation of tangent vectors.
   Two consecutive tangent vectors $\mathbf{v}(t_1)$ and $\mathbf{v}(t_2)$.
   Criterion: $\langle \mathbf{v}(t_1), \mathbf{v}(t_2) \rangle < 0 \Rightarrow \mathbf{v}(t) \perp t-\text{axis} \text{ for } t \in [t_1, t_2]$.
   Tangents are simple byproduct of predictor-corrector path tracker.

3. **Location:** shooting method for step size.
   Consider $\mathbf{x}(t) = \mathbf{x}(t_1) + h\, \mathbf{v}(t_1)$, find h and t: $\mathbf{v}(t) \perp t-\text{axis}$.
   Overshot turning point for $h = h_2$, at $\mathbf{x}(t_2)$ path has turned back.

Sweeping a Circle



Difficulties to Extend Approach

for any type of isolated singularity along a path

Detecting and locating quadratic turning points goes well.

Extending to any type of singularity has two difficulties:

1. detection: flip of tangent orientation no longer suffices
   $\rightarrow$ the path tracker glides over the singularity
2. location: higher order singularities may have corank > 1
   $\rightarrow$ the path tracker fails to converge

Solutions for these difficulties:

1. use a Jacobian criterion for detection, and
2. algebraic higher order predictor for location.

Common tool: Puiseux series expansion at a point along the path.

Neural Network Model

a family of polynomial systems for any dimension n

V.W. Noonburg. A neural network modeled by an adaptive Lotka-Volterra system. *SIAM J. Appl. Math.* 1989.

- Applying a sweep to the polynomial systems:

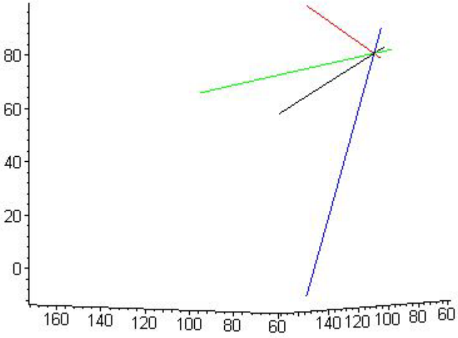
$$f(x, \lambda) = \begin{cases} x_1 x_2^2 + x_1 x_3^2 - \lambda x_1 + 1 = 0 \\ x_2 x_1^2 + x_2 x_3^2 - \lambda x_2 + 1 = 0 \\ x_3 x_1^2 + x_3 x_2^2 - \lambda x_3 + 1 = 0 \\ (\lambda + 1)(1 - t) + (\lambda - 1)t = 0 \end{cases}$$

- As t goes from 0 to 1, λ goes from -1 to $+1$.

- The tangent does not flip at the origin.
  The path tracker does not detect the quadruple point for $\lambda = 0$.

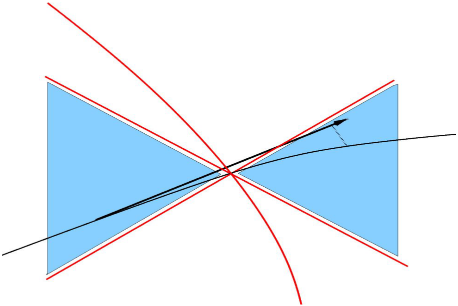
The Plot of Solution Paths for Neural Networks

the solution paths are really straight



Jumping Over Singularities

in case of jumping over a bifurcation point [Z. Mei]



The shaded blue part is the region where Newton's method converges.
On straight curves, the path tracker will never cut back its step size.

Puiseux or Fractional Power Series

expanding an algebraic curve at a point

The homotopy $h(\mathbf{x}, t) = \mathbf{0}$ defines solution paths $\mathbf{x}(t)$: $h(\mathbf{x}(t), t) \equiv \mathbf{0}$.

Because $\mathbf{x}(t)$ is an algebraic curve, at any point t_* the corresponding solution $\mathbf{x}(t_*) = \mathbf{z} = (z_1, z_2, \ldots, z_n)$ admits the expansion:

$$\left\{ \begin{array}{ll} x_k(s) = z_k s^{v_k}(1 + O(s)) & k = 1, 2, \ldots, n, v_k \in \mathbb{Z} \\ s^\omega = t - t_* & \text{as } t \rightarrow t_*, s \rightarrow 0 \end{array} \right.$$

Special case: $t_* = 0$: $s^\omega = t$ or $s = t^{1/\omega}$ and $x_k \rightarrow z_k t^{v_k/\omega}$ as $t \rightarrow 0$.

The ***winding number*** ω determines how hard the path curves.

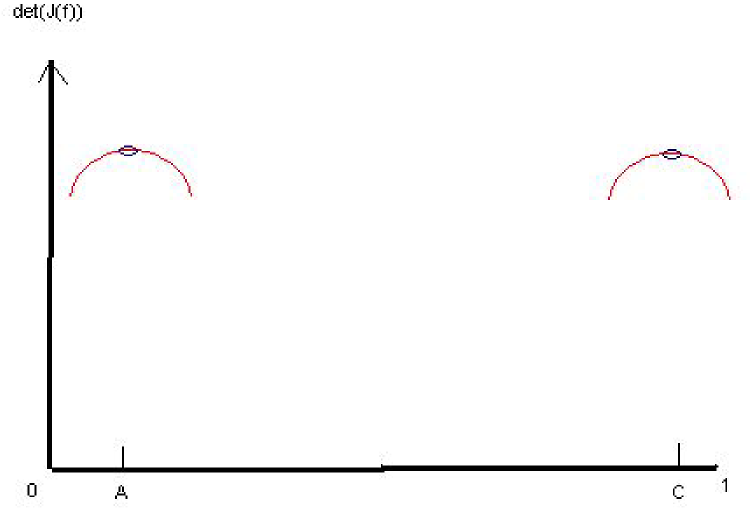
Determinant criterion for singularity along path $\mathbf{x}(t)$:

$$\text{singularity at } t_* \Leftrightarrow \det(A(\mathbf{x}(t_*))) = 0.$$

Via Puiseux series, determinant of Jacobian matrix is function of t.

Parabolic Interpolation of Determinants

monitor concavity of determinant as function of *t*



Parabolic Interpolation of Determinants

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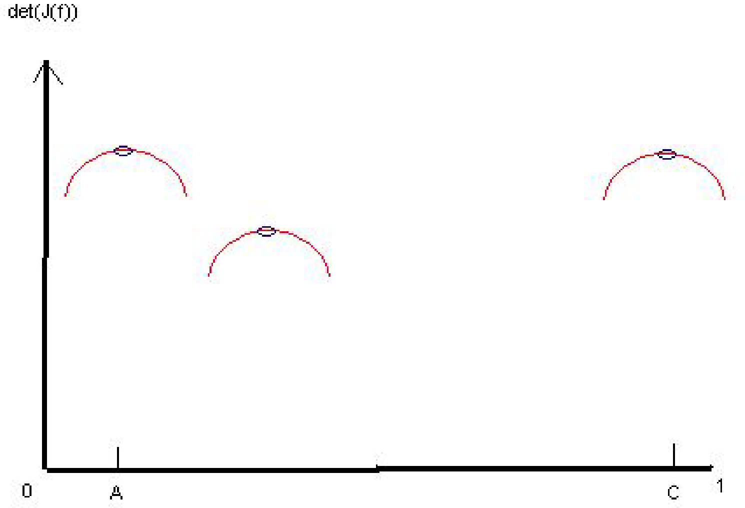

Parabolic Interpolation of Determinants

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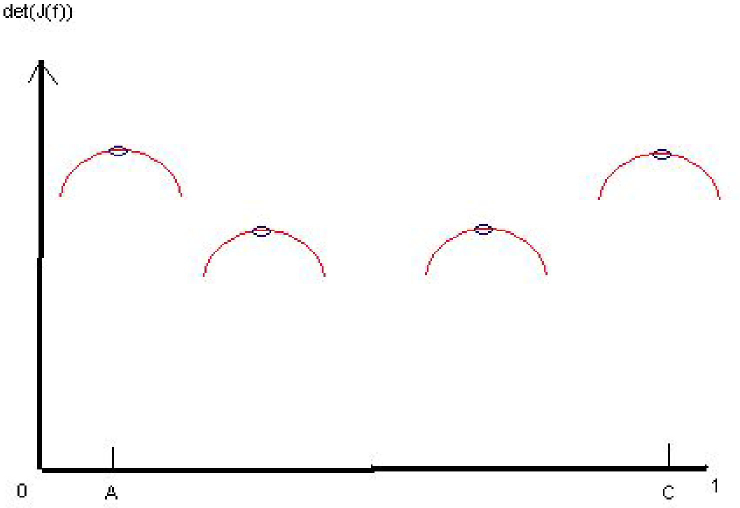
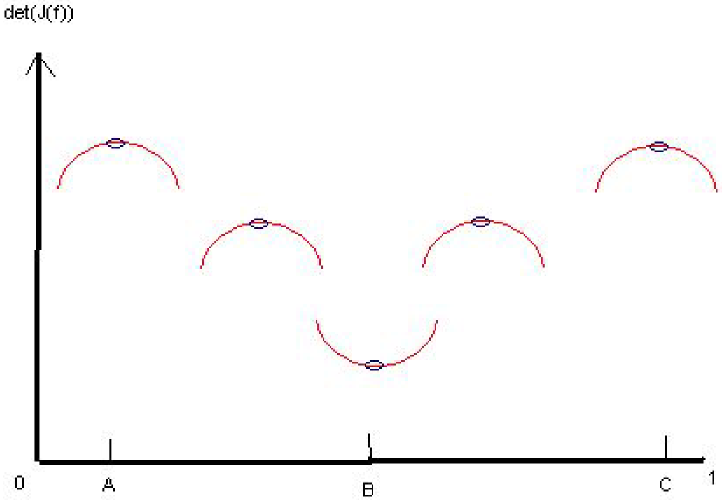


Parabolic Interpolation of Determinants

monitor concavity of determinant as function of t



Numerical Issues

implementing the parabolic interpolation criterion

Two important parameters:

- δ is the distance between two singularities: $|t_*^1 - t_*^2| > \delta$,
- h is the step size: $t_{m+1} = t_m + h$.

If $h \ll \delta$, then $\det(A(\mathbf{x}(t)))$ is unimodal in vicinity of singularities.

Because we work with polynomial systems,
we can bound the number of singularities.

Let $D = \displaystyle\prod_{k=1}^{n} \deg(f_k)$, the Bézout bound of $f(\mathbf{x}) = \mathbf{0}$, $f = (f_1, f_2, \ldots, f_n)$.

Then #singularities is at most D, counted with multiplicities.

Assuming uniform distribution of singularities ***(well conditioned)***,
a pessimistic lower bound on h is $1/D^2$.

our software: PHCpack

an open source software package for polynomial homotopy continuation

PHC = Polynomial Homotopy Continuation

- Version 1.0 archived as Algorithm 795 by ACM TOMS (1999)
- Pleasingly parallel implementations

  + **Yusong Wang** of Pieri homotopies (HPSEC'04)
  + **Anton Leykin** of monodromy factorization (HPSEC'05)
  + **Yan Zhuang** of polyhedral homotopies (HPSEC'06)
- Interactive Parallel Computing:

  + **Yun Guan:** PHClab, experiments with MPITB in Octave
  + **Kathy Piret:** bindings with Python, use of sockets
- Last major release v2.3 offered tools for computing a numerical irreducible decomposition and deflation of singularities.
- Release v2.3.37 on 2007-12-29: sweep in phc -p.

Release v2.3.42 extends **phcpy** and a preliminary **PHCwulf.py**.

Polynomial Systems

from the literature

1. Molecular Configurations:
   - **Emiris and Mourrain.** Computer algebra methods for studying and computing molecular conformations. *Algorithmica* 1999.
2. Neural Networks:
   - **V.W. Noonburg.** A neural network modeled by an adaptive Lotka-Volterra system. *SIAM J. Appl. Math.* 1989.
3. Symmetrical Stewart-Gough platforms:
   - **Yu Wang and Yi Wang.** Configuration Bifurcations Analysis of Six Degree-of-Freedom Symmetrical Stewart Parallel Mechanism. *Journal of Mechanical Design* 2005.

Polynomial Systems

the number of solutions in C^n for generic choices of parameters

Polynomial Systems	**n**	**#Solutions**
Molecular Configurations	3	16
Neural Networks	3	21
Neural Networks	4	73
Neural Networks	5	233
Neural Networks	10	59049
Neural Networks	15	14,348,907
Symmetrical Stewart-Gough Platforms	9	28 (real)

Table: Polynomial Systems which have higher-order multiple points

Molecular Configurations

applying the sweep homotopy algorithm to this system

- The system is small enough to handle with resultant/symbolic methods or global methods.
- Applying a sweep to molecular configurations:

$$
f(x,\lambda) = \begin{cases}
\frac{1}{2}(x_2^2 + 4x_2x_3 + x_3^2) + \lambda(x_2^2x_3^2 - 1) = 0 \\
\frac{1}{2}(x_3^2 + 4x_3x_1 + x_1^2) + \lambda(x_3^2x_1^2 - 1) = 0 \\
\frac{1}{2}(x_1^2 + 4x_1x_2 + x_2^2) + \lambda(x_1^2x_2^2 - 1) = 0 \\
(\lambda - 1)(1 - t) + (\lambda + 1)t = 0.
\end{cases}
$$

- The tangent flips at the higher-order turning point at the origin.
- For $\lambda = \pm 0.866025403780023$ on symmetrical curves of degree 6 and one of the eigenvalues of the Jacobian matrix changes signs.

Symmetrical Stewart-Gough platforms

nine quadratic polynomial equations

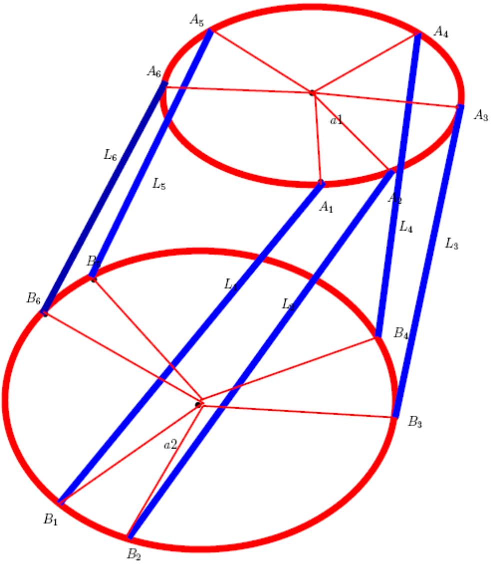
$$f(x, L_1) = \begin{cases} f_i = (x_i - x_{i0})^2 + (y_i - y_{i0})^2 + z_i^2 - L_i^2, i = 1, 2, \ldots, 6 \\ f_7 = (x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2 - 2R_1^2(1 - \beta)) \\ f_8 = (x_1 - x_0)^2 + (y_1 - y_0)^2 + (z_1 - z_0)^2 - R_1^2 \\ f_9 = (x_2 - x_0)^2 + (y_2 - y_0)^2 + (z_2 - z_0)^2 - R_1^2 \end{cases}$$

where

$$\begin{cases} x_i = w_1 x_0 + w_2^{m_1} w_3^{m_2} x_1 + w_2^{m_2} w_3^{m_1} x_2 \\ y_i = w_1 y_0 + w_2^{m_1} w_3^{m_2} y_1 + w_2^{m_2} w_3^{m_1} y_2 \\ z_i = w_1 z_0 + w_2^{m_1} w_3^{m_2} z_1 + w_2^{m_2} w_3^{m_1} z_2 \end{cases}$$

See Wang and Wang's paper for details of the system.

Symmetrical Stewart-Gough platforms



Computational Results

on the symmetrical Stewart-Gough platforms

- Applying the Jacobian criterion globally leads to an augmented system with a mixed volume equal to 4,608.
  Tracking 4,608 paths in 16 variables is much more expensive than tracking 512 paths in 9 variables.
  Sweeping to find all critical points works in a more efficient setup: at most 28 paths in 9 variables.

- By fixing $L_i, i = 2, 3, \ldots, 6$, to 1.5, 2.0, and 3.0, the sweep yields four special values for the natural parameter L_1 for each L_i.

- We have replicated the results from Wang and Wang's paper with higher precision than what they reported.
  In addition, z_0 can be either positive or negative.