Exploring the real parameter space

Margaret H. Regan

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Department of Mathematics and Computer Science
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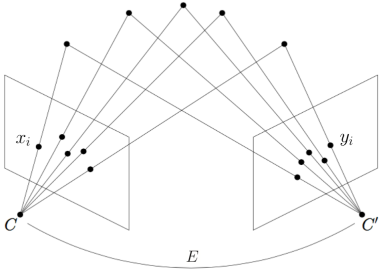
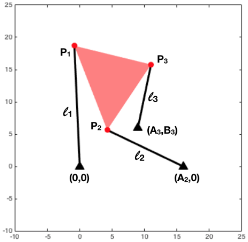
Outline

1. Introduction and motivation
   - Parameterized polynomial systems
2. Finding real solutions
   - Heuristically truncate
   - Real parameter homotopy
   - Real, positive solutions
3. Analyzing behavior of real solutions
4. Summary and future work

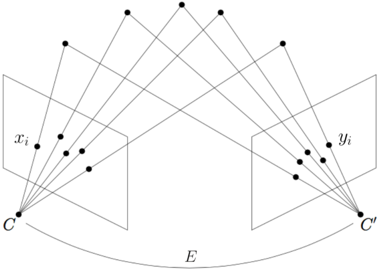
Parameterized polynomial systems

Many problems that arise in mathematics, science, and engineering can be formulated as solving a system of polynomial equations. These systems are generally dependent on a set of parameters.





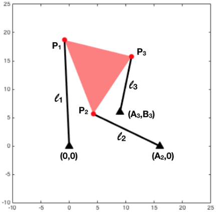
Example: 5-Point Problem



$$\begin{bmatrix} 2EE'E - \text{trace}(EE')E & \\ y_i'Ex_i & \text{for } i = 1:5 \end{bmatrix} \begin{matrix} \longleftarrow 9 \text{ polynomials} \\ \longleftarrow 5 \text{ polynomials} \end{matrix}$$

- E is a 3×3 matrix defined up to scale (in projective space).
- The parameters x_i and y_i are points in the plane.

Example: 3RPR mechanism



$$F(p,\phi;c) = \begin{bmatrix} \phi_1^2 + \phi_2^2 - 1 \\ p_1^2 + p_2^2 - 2(a_3p_1 + b_3p_2)\phi_1 + 2(b_3p_1 - a_3p_2)\phi_2 \\ \quad + a_3^2 + b_3^2 - c_1 \\ p_1^2 + p_2^2 - 2A_2p_1 + (a_2 - a_3)^2 + b_3^2 + A_2^2 - c_2 \\ \quad + 2((a_2 - a_3)p_1 - b_3p_2 + A_2a_3 - A_2a_2)\phi_1 \\ \quad + 2(b_3p_1 + (a_2 - a_3)p_2 - A_2b_3)\phi_2 \\ p_1^2 + p_2^2 - 2(A_3p_1 + B_3p_2) + A_3^2 + B_3^2 - c_3 \end{bmatrix}$$

Fix $c_3 = 100$ and consider ℓ_1 and ℓ_2 as paramters. At the "home" position $c^* = (75, 70)$, the system $F(p,\phi;c^*) = 0$ has 6 nonsingular real solutions.

Example: minimally bistable ERK subnetwork

$$\mathrm{S}_{00} + \mathrm{E} \xrightarrow{k_1} \mathrm{S}_{00}\mathrm{E} \xrightarrow{k_3} \mathrm{S}_{01}\mathrm{E} \xrightarrow{k_{\mathrm{cat}}} \mathrm{S}_{11} + \mathrm{E}$$

$$\mathrm{S}_{01}\mathrm{E} \underset{k_{\mathrm{on}}}{\overset{k_{\mathrm{off}}}{\rightleftharpoons}} \mathrm{S}_{01} + \mathrm{E}$$

$$\mathrm{S}_{10} + \mathrm{E} \xrightarrow{m_2} \mathrm{S}_{10}\mathrm{E} \xrightarrow{m_3} \mathrm{S}_{11} + \mathrm{E}$$

$$\mathrm{S}_{11} + \mathrm{F} \xrightarrow{\ell_1} \mathrm{S}_{11}\mathrm{F} \xrightarrow{\ell_3} \mathrm{S}_{10}\mathrm{F} \xrightarrow{\ell_{\mathrm{cat}}} \mathrm{S}_{00} + \mathrm{F}$$

$$\mathrm{S}_{10}\mathrm{F} \xrightarrow{\ell_{\mathrm{off}}} \mathrm{S}_{10} + \mathrm{F}$$

$$\mathrm{S}_{01} + \mathrm{F} \xrightarrow{n_1} \mathrm{S}_{01}\mathrm{F} \xrightarrow{n_3} \mathrm{S}_{00} + \mathrm{F}$$

Example: minimally bistable ERK subnetwork

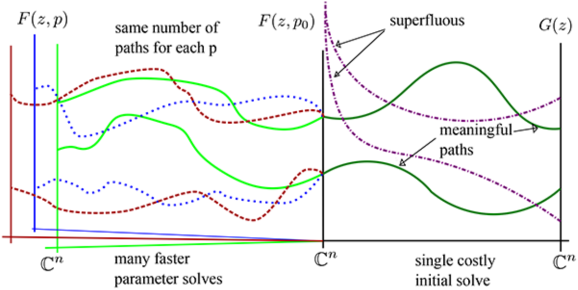
x_1	x_2	x_3	x_4	x_5	x_6	x_7	x_8	x_9	x_{10}	x_{11}	x_{12}
S_{00}	E	F	$S_{11}F$	$S_{10}F$	$S_{01}F$	$S_{01}E$	$S_{10}E$	S_{01}	S_{10}	$S_{00}E$	S_{11}

$$\begin{aligned}
x_1 + x_4 + x_5 + x_6 + x_7 + x_8 + x_9 + x_{10} + x_{11} + x_{12} &= S_{\text{tot}} &&=: c_1 \\
x_2 + x_7 + x_8 + x_{11} &= E_{\text{tot}} &&=: c_2 \\
x_3 + x_4 + x_5 + x_6 &= F_{\text{tot}} &&=: c_3.
\end{aligned}$$

$$\begin{aligned}
\dot{x_1} &= -k_1 x_1 x_2 + \ell_{\text{cat}} x_5 + n_3 x_6 &&=: f_1 \\
\dot{x_2} &= -k_1 x_1 x_2 - k_{\text{on}} x_2 x_9 - m_2 x_{10} x_2 + k_{\text{cat}} x_7 + k_{\text{off}} x_7 + m_3 x_8 &&=: f_2 \\
\dot{x_3} &= -\ell_1 x_3 x_{12} - n_1 x_3 x_9 + \ell_{\text{cat}} x_5 + \ell_{\text{off}} x_5 + n_3 x_6 &&=: f_3 \\
\dot{x_4} &= \ell_1 x_3 x_{12} - \ell_3 x_4 &&=: f_4 \\
\dot{x_5} &= \ell_3 x_4 - \ell_{\text{cat}} x_5 - \ell_{\text{off}} x_5 &&=: f_5 \\
\dot{x_6} &= n_1 x_3 x_9 - n_3 x_6 &&=: f_6 \\
\dot{x_7} &= k_{\text{on}} x_2 x_9 + k_3 x_{11} - k_{\text{cat}} x_7 - k_{\text{off}} x_7 &&=: f_7 \\
\dot{x_8} &= m_2 x_2 x_{10} - m_3 x_8 &&=: f_8 \\
\dot{x_9} &= -k_{\text{on}} x_2 x_9 - n_1 x_3 x_9 + k_{\text{off}} x_7 &&=: f_9 \\
\dot{x_{10}} &= -m_2 x_2 x_{10} + \ell_{\text{off}} x_5 &&=: f_{10} \\
\dot{x_{11}} &= k_1 x_1 x_2 - k_3 x_{11} &&=: f_{11} \\
\dot{x_{12}} &= -\ell_1 x_3 x_{12} + k_{\text{cat}} x_7 + m_3 x_8 &&=: f_{12}
\end{aligned}$$

(Parameter) homotopy continuation

How do we solve these systems?

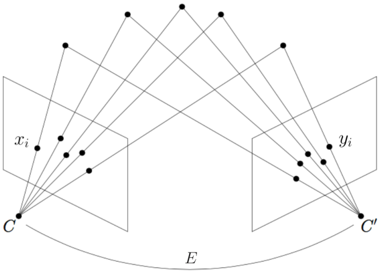


$$H(z,t) = F(z; t \cdot p_0 + (1-t) \cdot p)$$

- $F(z;p_0)$: start system
- $F(z;p)$: target system

Finding real solutions

5-point problem polynomial system



- The 5-point problem is a minimal problem with 10 solutions.
- **Goal:** To find the relationship between the data from the two cameras, i.e., solve for E.

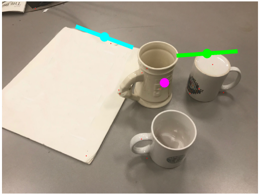
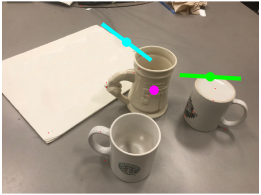
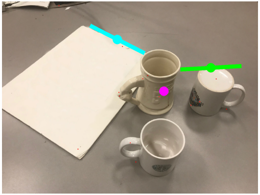
$$\begin{bmatrix} 2EE'E - \text{trace}(EE')E & \\ y_i' E x_i & \text{for } i = 1:5 \end{bmatrix} \begin{matrix} \longleftarrow 9 \text{ polynomials} \\ \longleftarrow 5 \text{ polynomials} \end{matrix}$$

Solving methods

- Gröbner basis methods and resultant based methods (Kúkelová, 2013)
- Specialized solvers based on the above symbolic methods
- Numerical homotopy continuation solvers
  - homotopycontinuation.jl, Bertini, M2
  - adaptive randomization algorithms
  - MINUS

Common theme: find all complex solutions, filter out the real solutions

Trifocal relative pose estimation

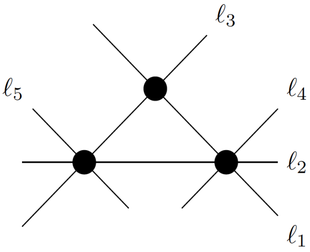




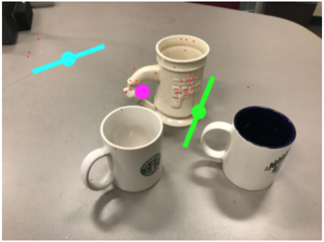
3-D reconstruction problems be difficult due to:

- too few features available/detected,
- repeated textures (e.g., brick walls) leading to ambiguously correlated features,
- blurred areas,
- and more.

We propose homotopy continuation techniques paired with additional attributes and more diverse features.

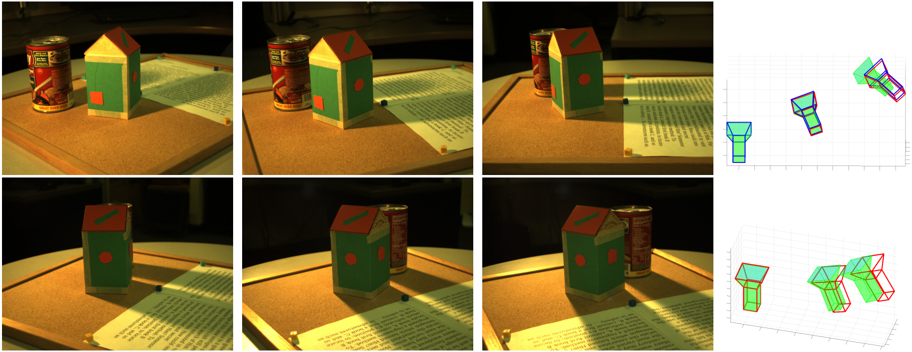
Example: Chicago





- The Chicago problem is a minimal problem with 312 solutions.
- Three cameras have data on three points and two lines (with constrained intersections) related to an object in space.
- Goal: to reconstruct the 3-D image based on the data from the three cameras.

Real data experiments



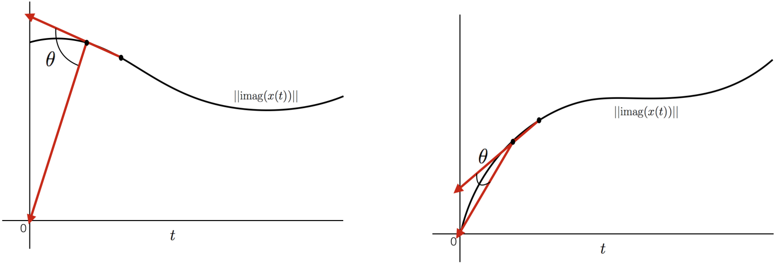
Samples of trifocal relative pose estimation of the Amsterdam Teahouse dataset. Top row is a sample triplet of images that COLMAP is able to tackle; second row is a triplet from the images where COLMAP fails. COLMAP results are in blue outlines, MINUS results are in red, and ground truth is green.

Heuristically truncate

Real solutions

For many real-world applications, only the real solutions are desired.

Q: Can we improve efficiency by just considering real solutions?



A: Yes! Use path data to terminate computations.

5-point Problem	Fixed	SVD	Leverage	Trunc.
Avg. # Steps	14.127	10.859	9.224	8.338

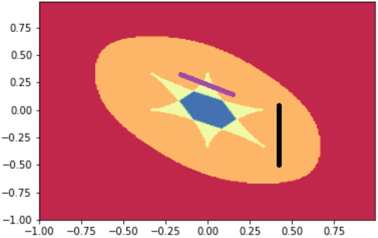
Challenges

- How do you know what angle value to use for the truncation?
- How do you know when to "test" this truncation, i.e., how close to $t = 0$?
- What information would you need to know about your system to determine a truncation heuristic and not leave out any real solutions?
- Is there a possible certification to indicate all real solutions have been found? That the meaningful/ground truth real solution is in the output?

Real parameter homotopy

Real parameter homotopy

It is possible to construct a real parameter homotopy within the complement of the discriminant locus.



With this discriminant locus input, we are able to track only real solution paths between real solutions.

Real parameter homotopy

- The classical parameter homotopy took 1.33 seconds on average.

Number of data points	Number of paths	Average time (in seconds)	Success rate
249	2	0.077	100%
26	4	0.081	100%
17	6	0.086	100%

Table: Average computation time for finding all real roots for the 3-oscillator Kuramoto model using a machine-learning-assisted real parameter homotopy method.

- For the 4-oscillator Kuramoto model the classical parameter homotopy completed in ~ 3.40 seconds vs. the real parameter homotopy of under ~ 0.15 seconds, with similar accuracy.

Challenges

- How do you know you have sampled densely enough?
- Sampling the discriminant locus...
- With 3 parameters this is difficult – how do we extrapolate to more?

Real, positive solutions

Minimally bistable ERK subnetwork

$$
\begin{aligned}
x_1 + x_4 + x_5 + x_6 + x_7 + x_8 + x_9 + x_{10} + x_{11} + x_{12} &= S_{\text{tot}} &=: c_1 \\
x_2 + x_7 + x_8 + x_{11} &= E_{\text{tot}} &=: c_2 \\
x_3 + x_4 + x_5 + x_6 &= F_{\text{tot}} &=: c_3.
\end{aligned}
$$

$$
\begin{aligned}
\dot{x_1} &= -k_1 x_1 x_2 + \ell_{\text{cat}} x_5 + n_3 x_6 &&=: f_1 \\
\dot{x_2} &= -k_1 x_1 x_2 - k_{\text{on}} x_2 x_9 - m_2 x_{10} x_2 + k_{\text{cat}} x_7 + k_{\text{off}} x_7 + m_3 x_8 &&=: f_2 \\
\dot{x_3} &= -\ell_1 x_3 x_{12} - n_1 x_3 x_9 + \ell_{\text{cat}} x_5 + \ell_{\text{off}} x_5 + n_3 x_6 &&=: f_3 \\
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\dot{x_5} &= \ell_3 x_4 - \ell_{\text{cat}} x_5 - \ell_{\text{off}} x_5 &&=: f_5 \\
\dot{x_6} &= n_1 x_3 x_9 - n_3 x_6 &&=: f_6 \\
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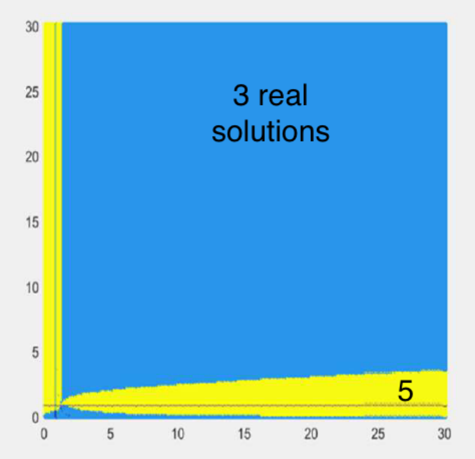
\end{aligned}
$$

Positive steady state solutions

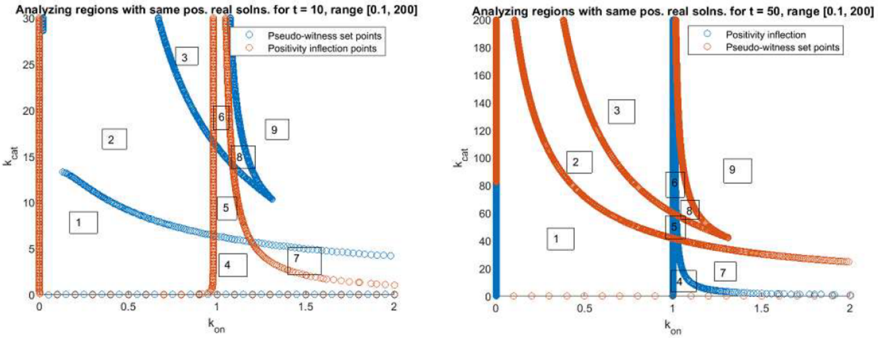
Keep k_{on} and k_{cat} left free and set all other parameters to 1.



With further analysis, 1 positive steady state found across parameter space.

Largest number?

Goal: Upper bound is 5 positive steady states – can we achieve this?
Conjecture: maximum is 3.



Here, founds regions for 3 positive steady states (1, 4, & 7), but is this a maximum? k_{on} and k_{cat} still free. Other parameters are parameterized with t from Newton polytope analysis.

Challenges

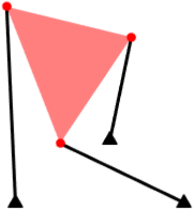
- What do we know about this parameterization from the Newton polytope? Does it automatically/theoretically yield the largest number of positive, real steady states?
- If not, how do we find a parameterization that does?
- Is it reasonable to assume that we have captured the infinite behavior?
- What to do if there are more parameters?
- Can we certify our sampling to know we know all components of the complement of the discriminant locus?

Analyzing behavior real of solutions

Kinematics

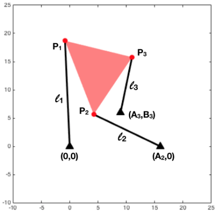
If we know the solutions, we can analyze the behavior of the solutions using parameter homotopy methods with data input.

Main question: How can we use data about the discriminant locus to determine how real solutions will interchange (real monodromy action)?



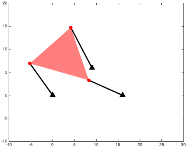
In kinematics, it is related to nonsingular assembly mode change for parallel manipulators.

3RPR mechanism

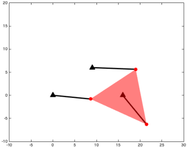


$$F(p,\phi;c) = \begin{bmatrix} \phi_1^2 + \phi_2^2 - 1 \\ p_1^2 + p_2^2 - 2(a_3 p_1 + b_3 p_2)\phi_1 + 2(b_3 p_1 - a_3 p_2)\phi_2 \\ \quad + a_3^2 + b_3^2 - c_1 \\ p_1^2 + p_2^2 - 2A_2 p_1 + (a_2 - a_3)^2 + b_3^2 + A_2^2 - c_2 \\ \quad + 2((a_2 - a_3)p_1 - b_3 p_2 + A_2 a_3 - A_2 a_2)\phi_1 \\ \quad + 2(b_3 p_1 + (a_2 - a_3)p_2 - A_2 b_3)\phi_2 \\ p_1^2 + p_2^2 - 2(A_3 p_1 + B_3 p_2) + A_3^2 + B_3^2 - c_3 \end{bmatrix}$$

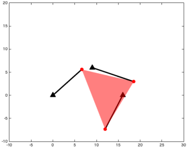
Fix $c_3 = 100$ and consider ℓ_1 and ℓ_2 as paramters. At the "home" position $c^* = (75, 70)$, the system $F(p,\phi;c^*) = 0$ has 6 nonsingular real solutions.



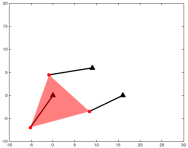
$x^{(1)}$



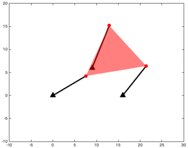
$x^{(2)}$



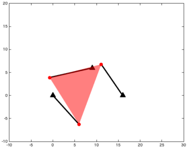
$x^{(3)}$



$x^{(4)}$



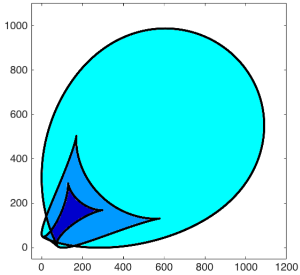
$x^{(5)}$



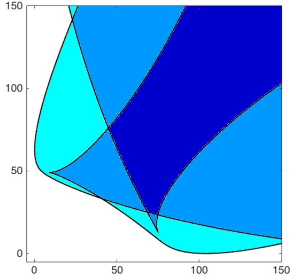
$x^{(6)}$

The 6 solutions to $F(p, \phi; c^*) = 0$.

3RPR mechanism



(a)

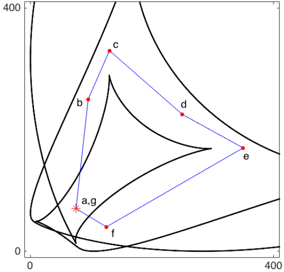


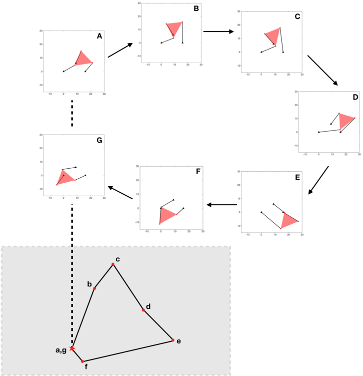
(b)

Regions of the parameter space $c = (c_1, c_2)$ colored by the number of real solutions where (a) is the full view and (b) is a zoomed in view of the lower left corner. The navy blue region has 6 real solutions, the grey blue region has 4 real solutions, the baby blue region has 2 real solutions, and the white region has 0 real solutions.

3RPR mechanism

Illustration of a nonsingular assembly mode change between $x^{(4)}$ and $x^{(5)}$.





Challenges

- How do we handle more than 2 parameters?
- How do we sample the discriminant locus?
- How do we know which monodromy loops to take?
- How do we know that the monodromy loops that we take have captured all behavior?

Summary and future work

Main goal:

- to work on theory and computation/analysis of problems involving real valued parameters and the impact on applications.

New directions:

- Parameter space exploration to determine the maximum number of real solutions or to map out regions of constant number of real solutions. *Applications:* kinematics, chemical reaction networks.
- Is there a way to determine whether a parameterized family of systems always has at least one real solution for every real set of parameters? *Applications:* computer vision.
- Can we decrease computational time and focus our methods only on the real solutions? How can we know ways in which to move around in our parameter space to acheive this?

- Adaptive strategies for solving parametrized systems using homotopy continuation → doi.org/10.1016/j.amc.2018.03.028
- TRPLP - Trifocal relative pose from lines at points → doi.org/10.1109/CVPR42600.2020.01209
- Machine learning the real discriminant locus → doi.org/10.1016/j.jsc.2022.08.001
- Real monodromy action → doi.org/10.1016/j.amc.2019.124983

Thank you!

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