Computational Algebraic Geometry

Numerical algebraic geometry

Kaie Kubjas

kaie.kubjas@aalto.fi

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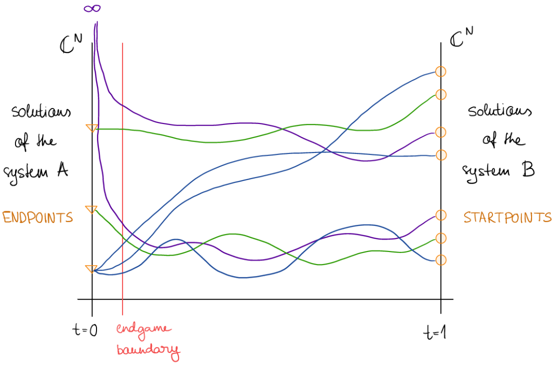
Overview

- Main goal: To solve a system of equations *A*.
- Take a similar system of equations *B* for which solutions are known.
- Deform the solutions of *B* to the solutions of *A*.
- This approach is called homotopy continuation.



Definitions

- A system of polynomial equations is called square if the number of equations is equal to the number of variables, i.e., the system has the form

$$f(z) := \begin{bmatrix} f_1(z_1, \dots, z_N) \\ \vdots \\ f_N(z_1, \dots, z_N) \end{bmatrix} = 0.$$

- We will first consider square systems and later explain how the results can be extended to general systems.

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- We will first consider square systems and later explain how the results can be extended to general systems.
- A solution $z^* \in \mathbb{C}^N$ is called isolated if it is the only solution in an open ball centered at z^*.

Intuition

Consider a square system

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1. Build and solve a start system $g(z)$.
   - $g(z)$ is related to $f(z)$: it usually has the same degrees
   - It should be easy to solve $g(z)$
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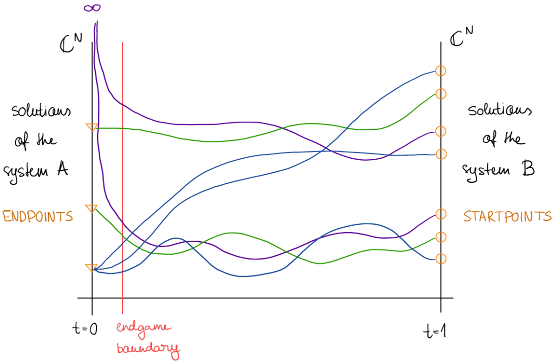
   - The solutions of $g(z)$ are called the startpoints
2. Construct a homotopy between $f(z)$ and $g(z)$.
   - Homotopy is a parametrized family of equations that specializes to $f(z)$ and $g(z)$ for different parameter values
   - The simplest homotopy is $H(z, t) = tg(z) + (1 - t)f(z)$, where t is a new parameter
   - $H(z, 1) = g(z)$ and $H(z, 0) = f(z)$

Intuition

3. Follow the solution paths from $t = 1$ to $t = 0$.
   - Predictor-corrector methods are used most of the way
   - Close to $t = 0$ more powerful endgames are used
   - Some paths could approach infinity as $t \to 0$; these paths are called divergent
   - Other paths can merge at $t = 0$



Example

We want to solve $f(z) = 0$ for the polynomial

$$f(z) = -2z^3 - 5z^2 + 4z + 1.$$

This particular example can be solved by the cubic formula. We consider it to illustrate the steps of the homotopy continuation.

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   - Any cubic polynomial with three distinct roots that can be solved easily.
   - We take $g(z) = z^3 + 1$.
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2. Homotopy
   - We choose linear homotopy $h(z, s) = sg(z) + (1 - s)f(z)$.
   - $h(z, 1) = g(z)$ and $h(z, 0) = f(z)$

3. **Follow the solution paths**
   - The variable s is complex, so there are infinitely many paths from 1 to 0.
   - Although the real line segment $[0, 1]$ seems like a natural choice, it can be problematic.
   - Instead consider the following family of circular arcs: Let $\gamma \in \mathbb{C} \backslash \mathbb{R}$. Then

$$q(t) = \frac{\gamma t}{\gamma t + (1 - t)}, \quad t \in [0, 1]$$

connects $s = 1$ to $s = 0$.

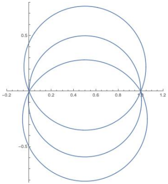


Figure: Plots are for six different values of γ.

Circular arcs

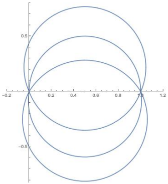


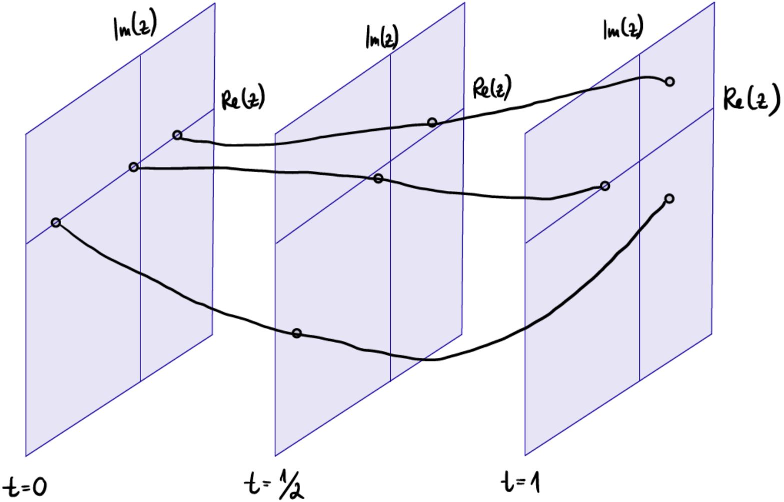
Figure: Plots are for six different values of γ.

- Following one of the arcs gives the homotopy $h(z, q(t)) = 0$.
- Substituting and clearing the denominators gives

$$H(z, t) = \gamma t g(z) + (1 - t) f(z).$$

- Choosing $\gamma = 0.40 + 0.77i$ gives three solution paths that never intersect.
- From $\mathbb{V}(g)$ we get $\mathbb{V}(f) = \{-3.0942, -0.2028, 0.7969\}$.

Example



Choice of γ

- If γ is chosen randomly in $\mathbb{C}$, then with probability one the homotopy defines three smooth paths.
- To see this, we consider the behavior of $h(z, s) = 0$ as s varies.
- For most $s^* \in \mathbb{C}$, $h(z, s^*) = 0$ is a cubic equation with three distinct roots.
- For a few s^* there are only two distinct solutions.
- The use of circular arcs to obtain a path between $s = 1$ and $s = 0$ and choosing γ randomly is known as the "gamma trick".

NumericalAlgebraicGeometry in Macaulay2

NAG-example.m2

```
needsPackage("NumericalAlgebraicGeometry")
R = CC[z];
F = {-2*z^3-5*z^2+4*z+1};
s = solveSystem F
realPoints s
```

```
U:**-  NAG-example.m2   All L5     (Macaulay2)
```

```
+ M2 --no-readline --print-width 140
Macaulay2, version 1.14
--loading configuration for package "FourTiTwo" from file /Users/kubjask1/Library/Application Support/Macaulay2/init-FourTiTwo.m2
--loading configuration for package "Topcom" from file /Users/kubjask1/Library/Application Support/Macaulay2/init-Topcom.m2
with packages: ConwayPolynomials, Elimination, IntegralClosure, InverseSystems, LLLBases, PrimaryDecomposition, ReesAlgebra, TangentCone,
               Truncations

i1 : needsPackage("NumericalAlgebraicGeometry")
--loading configuration for package "NumericalAlgebraicGeometry" from file /Users/kubjask1/Library/Application Support/Macaulay2/init-NumericalAlgebraicGeometry.m2
--loading configuration for package "PHCpack" from file /Users/kubjask1/Library/Application Support/Macaulay2/init-PHCpack.m2
--loading configuration for package "Bertini" from file /Users/kubjask1/Library/Application Support/Macaulay2/init-Bertini.m2

o1 = NumericalAlgebraicGeometry

o1 : Package

i2 : R = CC[z];

i3 : F = {-2*z^3-5*z^2+4*z+1};

i4 : s = solveSystem F

o4 = {{-3.09415}, {.796927}, {-.202773}}

o4 : List

i5 : realPoints s

o5 = {{-3.09415}, {.796927}, {-.202773}}

o5 : List

i6 : 
```

```
U:**-  *M2*        All L34    (Macaulay2 Interaction:run)
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Homotopy

Definition

Given two continuous functions $f, g : \mathbb{C}^N \to \mathbb{C}^N$, a homotopy is a continuous function

$$H(z,t) : \mathbb{C}^N \times [0,1] \to \mathbb{C}^N$$

satisfying $H(z,0) = f(z)$ and $H(z,1) = g(z)$.

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- For homotopy continuation, the homotopy H is obtained from composing the family of systems $\mathcal{H}(z; s)$ with a path $s = q(t)$.
- $\mathcal{H}(z; s) : \mathbb{C}^N \times U \to \mathbb{C}^N$, where $U \subseteq \mathbb{C}^M$ is an open set, $\mathcal{H}$ is polynomial in z and analytic in s
- $q : [0, 1] \to U$ is a differentiable map

Path tracking

Definition

Path tracking is the numerical process of approximating the paths from startpoints to endpoints.

Path tracking gives approximations of the solutions of $H(z, 0) = 0$ from the known solutions of $H(z, 1) = 0$.

Good homotopy

A good homotopy for

$$f(z) := \begin{bmatrix} f_1(z_1, \ldots, z_N) \\ \vdots \\ f_N(z_1, \ldots, z_N) \end{bmatrix} = 0$$

and a set of D distinct solutions S_1 of $g(z)$ is a system of infinitely differentiable functions

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1. for any $t \in [0, 1]$, $H(z, t)$ is a system of polynomials;
2. for any $w \in S_1$, there is a smooth map $p_j(t) : (0, 1] \to \mathbb{C}^N$ satisfying $p_j(1) = w$;

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3. the associated paths do not cross;
4. for each $t^* \in (0, 1]$ the points $p_j(t^*)$ are smooth isolated solutions of $H(z, t^*)$.

Good homotopy

Definition

We say that the above homotopy is a good homotopy for the system

$$f(z) := \begin{bmatrix} f_1(z_1, \ldots, z_N) \\ \vdots \\ f_N(z_1, \ldots, z_N) \end{bmatrix} = 0$$

if one can choose D distinct solutions S_1 of $g(z) = H(z, 1)$ such that the set

$$S_0 = \left\{ z \in \mathbb{C}^N : \|z\|_2 < \infty \text{ and } z = \lim_{t \to 0} p_j(t) \right\}$$

contains every isolated solution of $f(z) = 0$.

Theorem (Bezout's theorem)

Assume that the system of polynomial equations

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has finitely many solutions in $\mathbb{C}^N$*. Let* $d_i = \deg f_i$*. Then the system* f *has at most* $d_1 \cdots d_N$ *solutions.*

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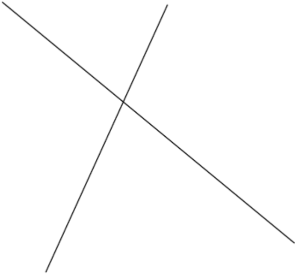
- For general systems of polynomial equations the number of solutions equals this bound.
- The Bernstein–Kushnirenko Theorem gives better upper bounds for special systems, but it is more complicated.

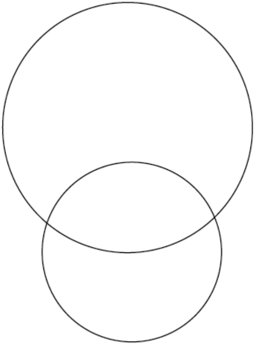
Bezout's theorem



$d_1 = d_2 = 1$

$d_1 \cdot d_2 = 1$

solutions $= 1$



$d_1 = d_2 = 2$

$d_1 \cdot d_2 = 4$

solutions $= 2$

Total-degree homotopies

We construct a good homotopy

$$H(z,t) = (1-t)\begin{bmatrix} f_1(z_1,\dots,z_N) \\ \vdots \\ f_N(z_1,\dots,z_N) \end{bmatrix} + \gamma t \begin{bmatrix} g_1(z_1,\dots,z_N) \\ \vdots \\ g_N(z_1,\dots,z_N) \end{bmatrix} = 0$$

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as follows:

- Let $d_i = \deg f_i$.
- Choose polynomials $g_1,\dots,g_N$ such that they have degrees $d_1,\dots,d_N$, the system $g(z)=0$ is easy to solve and it has exactly $D := d_1 d_2 \cdots d_N$ solutions.

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- For example, one can take $g_i(z) = z_i^{d_i} - 1$.
- In this case, the solution set of $g(z) = 0$ is given by

$$\left\{ \left(e^{(j_1/d_1)2\pi i}, \ldots, e^{(j_N/d_N)2\pi i} \right) : 0 \le j_i \le d_i \text{ for } i = 1, \ldots, N \right\}.$$

Total-degree homotopies

- Choose a random complex number $\gamma \neq 0$.
- In practice γ is chosen in a small band around the unit circle.
- If γ is chosen randomly, then with probability one we get a good homotopy.
- Total-degree homotopies are the simplest of all homotopies. Alternatively, one can use more special degree bounds.

Path tracking

Assume that we have:

- a family of functions on $\mathbb{C}^N$

$$H(z;q) = \begin{bmatrix} H_1(z_1,\ldots,z_N;q_1\ldots,q_M) \\ \vdots \\ H_N(z_1,\ldots,z_N;q_1\ldots,q_M) \end{bmatrix} = 0$$

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- differentiable maps $\phi : t \in [0,1] \to q \in \mathbb{C}^M$ and $\psi : t \in [0,1] \to z \in \mathbb{C}^N$ satisfying
  1. $H(\psi(t),\phi(t)) = 0$ for $t \in (0,1]$ and
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  2. the Jacobian of H with respect to $z_1,\dots,z_N$ has rank N for the points $(\psi(t),\phi(t))$ with $t \in (0,1]$.
- We construct H and ϕ in such a way that ψ exists and $\psi(1) = p_0$. The objective is to compute $p^* = \psi(0)$.

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- Differentiating $H(z(t), t) = 0$ with respect to t gives

$$\frac{\partial H(z(t),t)}{\partial t} + \sum_{i=1}^{N} \frac{\partial H(z(t),t)}{\partial z_i} \frac{dz_i(t)}{dt} = 0 \text{ with } z(1) = p_0.$$

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- Let $JH(z, t)$ denote the Jacobian matrix of H with respect to the variables z

$$JH := \frac{\partial H}{\partial z} := \begin{bmatrix} \frac{\partial H_1}{\partial z_1} & \cdots & \frac{\partial H_1}{\partial z_N} \\ \vdots & \ddots & \vdots \\ \frac{\partial H_N}{\partial z_1} & \cdots & \frac{\partial H_N}{\partial z_N} \end{bmatrix}$$

evaluated at (z, t) and let $z(t) = [z_1(t), \ldots, z_N(t)]^T$ denote the solution of the above differential equation.

Path tracking

- Using this notation, the above differential equation becomes

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- This is an initial value problem that can be solved using numerical methods.

First-order tracking

- We solve the initial value problem using Euler's method starting at $t_0 = 1$ with p_0 as the initial value and successively computing the approximations $p_1, p_2, \ldots$ at values $t_0 > t_1 > t_2 > \cdots > 0$.

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- The approximations are computed as

$$p_{i+1} = p_i - JH(p_i, t_i)^{-1} \frac{\partial H(p_i, t_i)}{\partial t} \Delta t_i,$$

where $\Delta t_i = t_{i+1} - t_i$.

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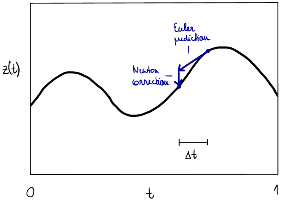
  where $\Delta t_i = t_{i+1} - t_i$.
- Geometrically this means predicting along the tangent line to the solution path at the current point of the path.



Correction

- The prediction is often followed by the correction using the Newton's method.
- This means Newton's method is used for $H(z, t_{i+1})$ starting with $z_0 = p_{i+1}$.
- Newton's method uses the iterative formula

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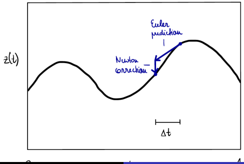
- This means Newton's method is used for $H(z, t_{i+1})$ starting with $z_0 = p_{i+1}$.
- Newton's method uses the iterative formula

$$z_{i+1} = z_i - [JH(z_i, t_{i+1})]^{-1} H(z_i, t).$$

- One or two iterations of Newton's method usually improves the prediction of $z(t_{i+1})$.
- p_{i+1} is replaced with the corrected value before starting the next predictor-corrector cycle.



Numerical methods

- In practice Δt_i is chosen adaptively.
- If the error after the correction is larger than the desired tracking accuracy, then Δt_i is halved.

Numerical methods

- In practice Δt_i is chosen adaptively.
- If the error after the correction is larger than the desired tracking accuracy, then Δt_i is halved.
- Often higher-order methods (e.g. Runge-Kutta methods) are used in practice.
- They have the advantage that they often allow larger step sizes.

From square systems to general systems

- Consider a general system

$$f(z) := \begin{bmatrix} f_1(z_1, \dots, z_N) \\ \vdots \\ f_n(z_1, \dots, z_N) \end{bmatrix} = 0.$$

- If $n < N$, then the system is underdetermined and the solution set has positive-dimensional solution components.

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$$f(z) := \begin{bmatrix} f_1(z_1, \ldots, z_N) \\ \vdots \\ f_n(z_1, \ldots, z_N) \end{bmatrix} = 0.$$

- If $n < N$, then the system is underdetermined and the solution set has positive-dimensional solution components.
- If $n > N$, let $A \in \mathbb{C}^{N \times n}$ be a random matrix. Instead of the system

$$f = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_n \end{bmatrix},$$

we consider the system

$$A \cdot f.$$

- Every polynomial in the system $A \cdot f$ has the form

$$a_{i1} f_1 + a_{i2} f_2 + \ldots + a_{in} f_n,$$

where a_{ij} are random complex numbers.

From square systems to general systems

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From square systems to general systems

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  where a_{ij} are random complex numbers.
- With probability one, all the isolated solutions of f are isolated solutions of $A \cdot f$.
- The system $A \cdot f$ could have more solutions than f.
- The extra solutions can be detected because they do not satisfy f.

From square systems to general systems

Example

- Let $p(z) = (z+1)(z-1)$ and $q(z) = z(z-1)$.
- The system $p(z) = q(z) = 0$ has one solution $z = 1$.

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$$2p(z) - 3q(z) = 2(z+1)(z-1) - 3z(z-1) = (2-z)(z-1).$$

- This system has two solutions $z = 1$ and $z = 2$.
- For $z = 2$, we have $p(2) = 3$ and $q(2) = 2$, so it is not a solution of the original system.

From square systems to general systems

Example

- Let $p(z) = (z+1)(z-1)$ and $q(z) = z(z-1)$.
- The system $p(z) = q(z) = 0$ has one solution $z = 1$.
- Consider

$$2p(z) - 3q(z) = 2(z+1)(z-1) - 3z(z-1) = (2-z)(z-1).$$

- This system has two solutions $z = 1$ and $z = 2$.
- For $z = 2$, we have $p(2) = 3$ and $q(2) = 2$, so it is not a solution of the original system.
- Since for most choices of constants we get a degree two polynomial, there are necessarily two solutions.
- This second solution changes when different coefficients are used.

Numerical algebraic geometry packages

- Bertini
- Julia Homotopy Continuation
- NumericalAlgebraicGeometry package in Macaulay2
- PHCpack

Julia Homotopy Continuation

juliahomotopycontinuation.org

An introduction to the numerical solution of polynomial systems

The basics of the theory and techniques behind HomotopyContinuation.jl

Conclusion

- Today's lecture was based on Chapter 2 in "Numerically Solving Polynomial Systems with Bertini" by Bates, Sommese, Hauenstein and Wampler.
- Exam will take place on Friday, February 26 at 13:00-17:00 in MyCourses. More information will be posted soon.
- Please fill out the course feedback form. You will get 1.5 extra points for filling it out.
- Check out the Algebraic Geometry I and II courses taught by Alexander Engström in the fall of 2021.
- Thank you for attending the course!!!