Diagonal Homotopies

This lecture is mainly based on [6] (see also [9]), where diagonal homotopies are defined to compute numerical representations (witness sets) of the intersection of positive dimensional solution sets. As application we consider the computation of the singular locus.

1 Intersecting Solution Sets

Consider the intersection two solution sets $A$ and $B$, given by their respective systems $f_A$ and $f_B$. For example: $A$ is the line $x_2 = 0$, defined as one of the solution components of $f_A(x_1, x_2) = x_1 x_2 = 0$; and $B$ is the line $x_1 - x_2 = 0$, defined as one of the solution components of $f_B = x_1(x_1 - x_2) = 0$. If we just stack the defining equations like

$$f(x) = \begin{cases} f_A = x_1 x_2 = 0 \\ f_B = x_1(x_1 - x_2) = 0 \end{cases}$$

then the problem is that $A \cap B = (0,0)$ does not occur as an irreducible solution component of $f^{-1}(0)$.

A more interesting example is the intersection of a sphere with a cylinder. The curve $C$ defined by this intersection is

$$C := \{ (x_1, x_2, x_3) \mid x_1^2 + x_2^2 - 1 = 0 \cap (1 + 0.5)^2 + x_2^2 + x_3^2 - 1 = 0 \}$$

and is depicted below.

The equations $f_A(x) = x_1^2 + x_2^2 - 1 = 0$ and $f_B(x) = (x_1 + 0.5)^2 + x_2^2 + x_3^2 - 1 = 0$ are part of a witness set representation of the cylinder and the sphere respectively. Both sets are two dimensional and of degree two. Each witness set contains two random hyperplanes and two points of intersection of these hyperplanes with the defining equations. As the input is given as two witness sets, the output consists also of witness sets.

The idea is to consider the product $A \times B$. Denote the intersecting hyperplanes for $A$ and $B$ respectively by $L_{A1}, L_{A2}$ and $L_{B1}, L_{B2}$. Then we use $u$ and $v$ for the coordinates of $A$ and $B$. A special instance of the diagonal homotopies is then

$$h(x, t) = (1 - t) \begin{pmatrix} f_A(u_1, u_2, u_3) = 0 \\ f_B(v_1, v_2, v_3) = 0 \\ L_{A1}(u_1, u_2, u_3) = 0 \\ L_{A2}(u_1, u_2, u_3) = 0 \\ L_{B1}(v_1, v_2, v_3) = 0 \\ L_{B2}(v_1, v_2, v_3) = 0 \end{pmatrix} + t \begin{pmatrix} f_A(u_1, u_2, u_3) = 0 \\ f_B(v_1, v_2, v_3) = 0 \\ u_1 - v_1 = 0 \\ u_2 - v_2 = 0 \\ u_3 - v_3 = 0 \\ L_{AB}(u_1, u_2, u_3) = 0 \end{pmatrix}.$$ (3)

As $t$ goes from 0 to 1, the deformation starts at pairs $(\alpha, \beta) \in A \times B$, where $\alpha$ and $\beta$ are witness point on $A$ and $B$ respectively satisfying $f_A(\alpha) = 0$, $f_B(\beta) = 0$ and $L_{A1}(\alpha) = 0 = L_{A2}(\alpha)$, $L_{B1}(\beta) = 0 = L_{B2}(\beta)$. At $t = 1$ we find witness points on the curve of intersection.
2 The Singular Locus

Given a system \( f(x) = 0 \). The singular locus of its solution set \( f^{-1}(0) \) is where the Jacobian matrix \( J_f(x) \) of \( f \) is singular. Using \( n \) auxiliary multipliers \( \lambda \), we consider the intersection of \( A = f^{-1}(0) \) with the solution set \( B \) of the system

\[
\begin{align*}
J_f(x)\lambda &= 0 \\
h^T\lambda &= 1
\end{align*}
\]

where \( h \) is a random vector of complex coefficients to scale the multiplier coefficients in the combinations of the columns of the Jacobian matrix.

The system below is mentioned as a nontrivial example in [10, §9.4.3, page 391] and comes from molecular chemistry [1]:

\[
f(x,a) = \begin{cases} 
\frac{1}{2}(x_2^2 + 4x_2x_3 + x_3^3) + a(x_2^2x_3^2 - 1) = 0 \\
\frac{1}{2}(x_3^2 + 4x_3x_1 + x_1^3) + a(x_3^2x_1^2 - 1) = 0 \\
\frac{1}{2}(x_1^2 + 4x_1x_2 + x_2^3) + a(x_1^2x_2^2 - 1) = 0.
\end{cases}
\]

For generic choices of the parameter \( a \), the system \( f(x,a) = 0 \) has 16 isolated solutions. Via (4) we compute those values for \( a \) for which \( f(x,a) = 0 \) has isolated singularities or positive dimensional solution sets.

3 Solving Systems restricted to an Algebraic Set

In this section, we consider a generalization of coefficient-parameter homotopies. Consider \( f(x,y) = 0 \) over \( X \times Y \), where \( Y \) is the parameter space. We want the solutions to \( f(x,y^*) = 0 \), for some \( y^* \in Y \).

1. Choose a general \( y' \in Y \) (\( y' \neq y^* \)). \( D = \#\{ x \mid f(x,y') = 0 \} \) is maximal for all \( y' \in Y \).

2. Construct a curve \( B \subset Y \) connecting \( y' \) to \( y^* \).

3. Construct a map \( c: [0,1] \times \Gamma \rightarrow B \), \( \Gamma = \{ \gamma \in \mathbb{C} \mid |\gamma| = 1 \} \), so that \( c(0,\Gamma) = y' \) and \( c(1,\Gamma) = y^* \).

4. Choose \( \gamma \in \Gamma \) at random and track \( D \) solution paths defined by the homotopy \( f(x,c(t,\gamma)) = 0 \), starting at \( t = 0 \) at the solutions of \( f(x,y') = 0 \) and ending at \( t = 1 \) at the desired solutions of \( f(x,y^*) = 0 \).

Also the cascade of homotopies is generalized. In this abstract setting we consider \( X \) as reduced pure \( n \)-dimensional algebraic set (abstract means: no equations specified for \( X \)) and we consider \( f \) in a cascade of embeddings \( \mathcal{E}_n(f) = \mathcal{E}(f) \) and \( \mathcal{E}_0(f) = f \), where \( \mathcal{E}_i(f) \) is restricted to \( Y_i \).

\[
\mathcal{E}(f,x,z,Y) = \begin{bmatrix} f(x) + A_1^Tz \\
z - A_0 - A_1x \end{bmatrix} \quad Y = \begin{bmatrix} (A_0, A_1, A_2), A_0 \in \mathbb{C}^{n\times 1}, & A_1 \in \mathbb{C}^{n\times n}, & A_2 \in \mathbb{C}^{n\times n} \end{bmatrix}
\]

The stratification of the parameter space is \( Y_0 \subset Y_1 \subset \cdots \subset Y_n \), last \( N - i \) rows of \( Y_i \) are zero. In practice we replace \( n \) by the top dimension of the solution set plus one.

For random \( \gamma_i \in \mathbb{C}, |\gamma_i| = 1 \), the homotopy

\[
H_i(x,z,t,Y,\gamma_i) = \gamma_i (1 - t) \mathcal{E}_i(f)(x,z,Y) + t \left( \mathcal{E}_{i-1}(f)(x,z,Y_{i-1}) \right)
\]

defines paths starting at \( t = 0 \) at the solutions of \( \mathcal{E}_i(f) \), ending at \( t = 1 \) at the solutions of \( \mathcal{E}_{i-1}(f) \).

**Theorem 3.1** For the homotopy (7), the following holds:

1. Solutions of \( H_i(x,z,t = 0,Y,\gamma_i) = 0 \) with \( z = (z_1, z_2, \ldots, z_i) \neq 0 \) are regular, and stay regular for all \( t < 1 \).

2. Solutions of \( H_i(x,z,t = 1,Y,\gamma_i) = 0 \) contain all witness sets on the \((i - 1)\)-dimensional components of \( f^{-1}(0) \).
4 Homotopies to Intersect Solution Sets

Given two irreducible components $A$ and $B$ in $\mathbb{C}^n$, we consider their product $X := A \times B \subset \mathbb{C}^{n+n}$. Then $A \cap B \cong X \cap \Delta$ where $\Delta$ is the diagonal of $\mathbb{C}^{n+n}$ defined by

$$\delta(u, v) := \begin{bmatrix} u_1 - v_1 = 0 \\ u_2 - v_2 = 0 \\ \vdots \\ u_n - v_n = 0 \end{bmatrix}$$ on $X$.

Notice that $\delta$ plays role of $f$ in the abstract embedding.

The input data for the diagonal homotopies is

Let $A \in \mathbb{C}^n$ be an irreducible component of $f_A^{-1}(0)$, $\dim A = a$; and $B \in \mathbb{C}^n$ be an irreducible component of $f_B^{-1}(0)$, $\dim B = b$.

Assuming $a \geq b$ and $B \not\subseteq A$, then $\dim(A \cap B) \leq b - 1$. To represent $A$ and $B$ as complete intersections, we may randomize the equations: $F_A(u) := \mathcal{R}(f_A, n-a)$ and $F_B(v) := \mathcal{R}(f_B, n-b)$. After these randomizations, $A \times B$ is a solution component of $\mathcal{F}(u, v) := \begin{bmatrix} F_A(u) \\ F_B(v) \end{bmatrix} = 0$.

Let $\{\alpha_1, \alpha_2, \ldots, \alpha_{\deg A}\}$ satisfy $F_A(u) = 0$ and $L_A(u) = 0$; and $\{\beta_1, \beta_2, \ldots, \beta_{\deg B}\}$ satisfy $F_B(v) = 0$ and $L_B(v) = 0$, where $L_A(u) = 0$ is a system of $a$ general hyperplanes; and $L_B(v) = 0$ is a system of $b$ general hyperplanes. We now distinguish two cases, depending whether $a + b < n$ or $a + b \geq n$.

1. When $a + b < n$, randomize the diagonal $D(u, v) := \mathcal{R}(\delta(u, v), a+b)$.

   At the start of the cascade (denote $z_{1:b} = (z_1, z_2, \ldots, z_b)^T$):

   $$E_b(u, v, z_{1:b}) = \begin{bmatrix} \mathcal{F}(u, v) \\ \mathcal{R}(D(u, v), z_1, \ldots, z_b; a+b) \\ z_{1:b} - \mathcal{R}(1, u, v; b) \end{bmatrix} = 0. \quad (8)$$

   The homotopy

   $$\begin{bmatrix} (1-t) \gamma & \mathcal{F}(u, v) \\ L_A(u) \\ L_B(v) \\ z_{1:b} \end{bmatrix} + t E_b(u, v, z_{1:b}) = 0 \quad (9)$$

   starts the cascade at $t = 0$, at the deg $A \times \deg B$ solutions, at the product $\{(\alpha_1, \beta_1), (\alpha_1, \beta_2), \ldots, (\alpha_{\deg A}, \beta_{\deg B})\} \subset \mathbb{C}^{2n}$.

2. When $a + b \geq n$, as $A \cap B \neq \emptyset \Rightarrow \dim(A \cap B) \geq a + b - n$, the cascade starts at

   $$E_b(u, v, z_{(a+b-n+1):b}) = \begin{bmatrix} \mathcal{F}(u, v) \\ \mathcal{R}(\delta(u, v), z_{a+b-n+1}, \ldots, z_b; n) \\ \mathcal{R}(1, u, v; a+b-n) \\ z_{(a+b-n+1):b} - \mathcal{R}(1, u, v; n-a) \end{bmatrix} = 0, \quad (10)$$

   where $z_{(a+b-n+1):b} = (z_{a+b-n+1}, \ldots, z_b)^T$. Use

   $$\begin{bmatrix} (1-t) \gamma & \mathcal{F}(u, v) \\ L_A(u) \\ L_B(v) \\ z_{(a+b-n+1):b} \end{bmatrix} + t E_b(u, v, z_{(a+b-n+1):b}) = 0 \quad (11)$$

   as before to start the cascade at $t = 0$. 

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5 an illustrative example

The diagonal homotopies lead to an equation-by-equation solver, which we illustrate on the following example:

\[ f = \begin{bmatrix} (y - x^2)(x^2 + y^2 + z^2 - 1)(x - 0.5) \\ (z - x^3)(x^2 + y^2 + z^2 - 1)(y - 0.5) \\ (y - x^2)(z - x^3)(x^2 + y^2 + z^2 - 1)(z - 0.5) \end{bmatrix} . \]  

(12)

This example has been constructed in a factored form so that it is easy to identify the decomposition of \( Z = f^{-1}(0) \) into its irreducible solution components, as

\[ Z = Z_2 \cup Z_1 \cup Z_0 = \{ Z_{21} \} \cup \{ Z_{11} \cup Z_{12} \cup Z_{13} \cup Z_{14} \} \cup \{ Z_{01} \} \]  

(13)

where

1. \( Z_{21} \) is the sphere \( x^2 + y^2 + z^2 - 1 = 0 \),
2. \( Z_{11} \) is the line \( (x = 0.5, z = 0.5) \),
3. \( Z_{12} \) is the line \( (x = \sqrt{0.5}, y = 0.5) \),
4. \( Z_{13} \) is the line \( (x = -\sqrt{0.5}, y = 0.5) \),
5. \( Z_{14} \) is the twisted cubic \( (y - x^2 = 0, z - x^3 = 0) \),
6. \( Z_{01} \) is the point \( (x = 0.5, y = 0.5, z = 0.5) \).

The flow of the data in our algorithm is illustrated by Figure 1. The levels correspond to the dimensions of the solution components.

![Figure 1: Flow chart to compute witness points on all components for the illustrative example. The dangling arrows at the far right point to further filtering and factoring.](image)

at level 2: We first find the sphere as a common component of the first two equations, represented by two witness points which satisfy the third equation. The two witness points which are common to the two equations are removed from the list of points used to form start solutions in the diagonal homotopy at level 1.
at level 1: The diagonal homotopy traces twelve paths. Five paths diverge to infinity. The end points of six paths satisfy the third equation. These six end points are witness points on the components of dimension one: three lines and the twisted cubic. We take the point which does not satisfy the third equation to the next level down. It will serve to form start solutions in the diagonal homotopy at level 2.

at level 0: We intersect the third equation with the same line used to find the witness points on the hypersurfaces defined by the first two equations. In this way we immediately recognize the two points on the sphere. After removal of those two points, we have six (deg($f_3$) = 8) witness points left to form start solutions in the diagonal homotopy. Two paths diverge to infinity. Among the four other paths, one of them converged to the isolated solution.

6 Solving Subsystem by Subsystem

The diagonal homotopy leads to a doubling of the number of variables and to an increase in the complexity of the linear algebra operations during path following. Instead of this extrinsic representation of the solution sets, we can work with intrinsic coordinates. Consider for example the intrinsic coordinate representation of a hypersurface given by one polynomial $f$ in $n$ variables:

$$
\begin{align*}
\begin{cases}
f(x_1, x_2, \ldots, x_n) &= 0 \\
c_{1,0} + c_{1,1}x_1 + c_{1,2}x_2 + \cdots + c_{1,n}x_n &= 0 \\
c_{2,0} + c_{2,1}x_1 + c_{2,2}x_2 + \cdots + c_{2,n}x_n &= 0 \\
&\vdots \\
c_{n-1,0} + c_{n-1,1}x_1 + c_{n-1,2}x_2 + \cdots + c_{n-1,n}x_n &= 0
\end{cases}
\end{align*}
$$

At the left of (14) we see the system to compute the witness points on the hypersurface $f^{-1}(0)$. Instead of working in $\mathbb{C}^n$, we select a random offset vector $b$ and a general direction $v$. Then to compute witness points on the hypersurface, it suffices to solve a polynomial in one variable $\lambda$: $f(b + \lambda v) = 0$.

The cascade to intersect solution sets using intrinsic coordinate representations is developed in [7]. The benefit of working with the intrinsic representation is the reduction of the dimension of the linear algebra to the codimension of the solution sets. For example, a three dimensional solution set in $\mathbb{C}^{20}$ is parameterized by three variables, instead of 20. Intrinsic coordinates also eliminate the use of slack variables.

The diagonal homotopies give way to a more flexible way of solving polynomial systems. For example, one could develop a divide-and-conquer strategy, recursively partitioning the input equations, solving the smaller parts first, and then intersecting the computed witness sets. This numerical strategy is described in [8]. Symbolic algorithms to incrementally solve polynomial systems originated in [4] and [5]. Also the Gröbner free algorithms to compute geometric resolution with lifting fibers [3] gradually build up the solution sets of a polynomial system. Last and certainly not least, Gröbner basis algorithms [2] benefit from the assumption that the input polynomials form a regular sequence.

7 Exercises

1. Consider the intersection of $\{x = 0, y = 0\}$ with $\{z = 0, w = 0\}$.

    Describe how the diagonal homotopy works for this example.

2. Set up the system (4 for the nontrivial example (5). Use the diagonal homotopies available in \texttt{phc -c} to compute the singular values for $a$. Compute a witness set for those $a$ which lead to positive dimensional solution sets. Apply deflation to treat isolated singular solutions.

3. Give algorithms to define the linear algebra operations to convert between extrinsic and intrinsic coordinate representations of witness sets for hypersurfaces, as sketched in (14).
References


