Bernshteĭn's Second Theorem

1. Solutions at Infinity
   - there is more than one infinity
   - weighted projective space
2. Mass Action Kinetics
   - modeling chemical reactions
3. Bernshteĭn's Second Theorem
   - faces of polytopes and initial forms
   - Puiseux series and initial forms
4. Richardson Extrapolation
   - computing Puiseux series of diverging paths

MCS 563 Lecture 18
Analytic Symbolic Computation
Jan Verschelde, 23 February 2011

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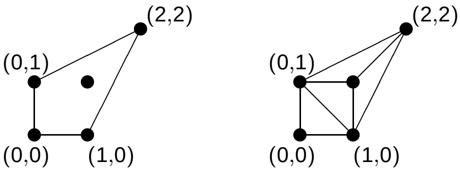
a polynomial system

$$f(\mathbf{x}) = \begin{cases} x_1^2x_2^2 + x_1x_2 + x_1 + x_2 + 1 = 0 \\ x_1^2x_2^2 - x_1x_2 + x_1 + x_2 - 1 = 0. \end{cases}$$

Subtracting the equations gives $x_1x_2 + 1 = 0$. Substituting then $x_2 = 1/x_1$ leads to a quadric, so we have 2 solutions.

$A = \{(2,2),(1,1),(1,0),(0,1),(0,0)\}$ is the support of the polynomials and a triangulation is below:



Kushnirenko's theorem applies: at most 4 solutions.

projective coordinates

For solutions at ∞ we use projective coordinates.

Replacing x_1 by z_1/z_0 and x_2 by z_2/z_0 leads
— after multiplication by z_0^4 — to

$$f([z_0 : z_1 : z_2]) = \begin{cases} z_1^2 z_2^2 + z_0^2 z_1 z_2 + z_0^3 z_1 + z_0^3 z_2 + z_0^4 = 0 \\ z_1^2 z_2^2 - z_0^2 z_1 z_2 + z_0^3 z_1 + z_0^3 z_2 - z_0^4 = 0. \end{cases}$$

Solutions at ∞ are solutions $\mathbf{z} \neq 0$ with $z_0 = 0$.

We see that only $z_1^2 z_2^2 = 0$ remains, or equivalently we find $[0 : 1 : 0]$ and $[0 : 0 : 1]$ representing two distinct solutions at infinity, but each with multiplicity two.

This is unsatisfactory, we want 2, not 4 solutions at ∞.

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Two Lines at ∞

The projective transformation $x_1 = z_1 z_0^{-1}$ and $x_2 = z_2 z_0^{-1}$ assumes one line at infinity, defined by $z_0 = 0$.

Exponents of z_0 in this transformation $-1, -1$ form the inner normal $(-1, -1)$ to the edge of the Newton polygon on which the highest degree monomials are supported.

Let us look at the edge with inner normal $(-2, +1)$ and use the coordinate transformation $x_1 = z_1 z_0^{-2}$ and $x_2 = z_2 z_0^{+1}$.

After this substitution and multiplication by z_0^2 we then find:

$$f([z_0 : z_1 : z_2]) = \begin{cases} z_1^2 z_2^2 + z_0 z_1 z_2 + z_1 + z_0^3 z_2 + z_0^2 = 0 \\ z_1^2 z_2^2 - z_0 z_1 z_2 + z_1 + z_0^3 z_2 - z_0^2 = 0. \end{cases}$$

Weighted Projective Space

$$f([z_0 : z_1 : z_2]) = \begin{cases} z_1^2 z_2^2 + z_0 z_1 z_2 + z_1 + z_0^3 z_2 + z_0^2 = 0 \\ z_1^2 z_2^2 - z_0 z_1 z_2 + z_1 + z_0^3 z_2 - z_0^2 = 0. \end{cases}$$

Setting $z_0 = 0$ now leaves us with $z_1^2 z_2^2 + z_1 = 0$ and we then find one solution at infinity: $[0 : -1 : 1]$.

The other solution at infinity is found via the projective transformation defined by the inner normal $(+1, -2)$.

This example has shown us that solutions at infinity are solutions of polynomial systems supported on faces of the Newton polytopes of the original system.

This compactification uses a weighted projective space.

Bernhteĭn's Second Theorem

chemical reactions

The equations to compute the steady states of an oxidation of H_2 on a catalytic surface yield the system

$$f(\mathbf{x}) = \left\{ \begin{array}{c} -k_{2,1}x_1x_2^2 - 2k_{10,7}x_1^2 + 2k_{7,10}x_5^2 = 0 \\ -2k_{2,1}x_1x_2^2 - 2k_{9,3}x_2^2 - 2k_{11,8}x_2x_4 + 2k_{3,9}x_5 = 0 \\ k_{2,1}x_1x_2^2 + (-k_{5,4} - k_{9,4})x_3 = 0 \\ k_{5,4}x_3 - 2k_{10,6}x_4^2 - 2k_{11,8}x_2x_4 = 0 \\ k_{2,1}x_1x_2^2 + k_{9,3}x_2^2 + k_{9,4}x_3 + 2k_{10,6}x_4^2 \\ +2k_{10,7}x_1^2 + 3k_{11,8}x_2x_4 - k_{3,9}x_5 - 2k_{7,10}x_5^2 = 0 \end{array} \right.$$

where x_1, x_2, x_3, and x_4 are the concentrations of O, H, H_2O, and H_2O_f; and x_5 is the amount of free space. The parameters $k_{i,j} > 0$ are rate constants. Add one conservation law: $2x_1 + x_2 + 2x_3 + 2x_4 + 2x_5 - c_1 = 0$.

matrix form

$$\begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & -2 & 2 & 0 \\ -2 & -2 & 2 & 0 & 0 & 0 & 0 & 0 & -2 \\ 1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & -2 \\ 1 & 1 & -1 & 1 & 0 & 2 & 2 & -2 & 3 \end{bmatrix} \begin{bmatrix} k_{2,1} & x_1 x_2^2 \\ k_{9,3} & x_2^2 \\ k_{3,9} & x_5 \\ k_{9,4} & x_3 \\ k_{5,4} & x_3 \\ k_{10,6} & x_4^2 \\ k_{10,7} & x_1^2 \\ k_{7,10} & x_5^2 \\ k_{11,8} & x_2 x_4 \end{bmatrix} = \mathbf{0}$$

Drawbacks: same columns of coefficient matrix (except for sign), monomials appear twice with different constants.

modeling with graphs

Using a directed weighted bipartite graph the system is

$$f(\mathbf{x}) = \begin{cases} Y_s I_a I_K \Psi(\mathbf{x}) = \mathbf{0} \\ 2x_1 + x_2 + 2x_3 + 2x_4 + 2x_5 - c_1 = 0. \end{cases}$$

where I_a and I_K are incidence matrices,

$$Y_s = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \end{bmatrix}$$

and $\Psi(\mathbf{x}) = \left(x_1x_2^2, x_3x_5, x_2^2, x_3, x_4, x_4^2, x_1^2, x_2x_4, x_5, x_5^2, x_5^3\right)^T$.

#monomials in $\Psi(\mathbf{x})$ equals the number of complexes.

Bernhteĭn's Second Theorem

initial forms

The ith equation of $f(\mathbf{x}) = \mathbf{0}$ has support A_i:

$$f_i(\mathbf{x}) = \sum_{\mathbf{a} \in A_i} c_{i\mathbf{a}} \mathbf{x}^{\mathbf{a}}, \quad c_{i\mathbf{a}} \in \mathbb{C}^*, \quad \mathbf{x}^{\mathbf{a}} = x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n},$$

and its Newton polytope is $P_i := \mathrm{conv}(A_i)$.

For any $\mathbf{v} \neq \mathbf{0}$, the face $\partial_{\mathbf{v}} P_i$ of P_i is spanned by

$$\partial_{\mathbf{v}} A_i := \{ \mathbf{a} \in A_i \mid \langle \mathbf{a}, \mathbf{v} \rangle = \min_{\mathbf{a}' \in A_i} \langle \mathbf{a}', \mathbf{v} \rangle \}.$$

The set $\partial_{\mathbf{v}} A_i$ is the support of the initial form of f_i in the direction $\mathbf{v}$:

$$\mathrm{in}_{\mathbf{v}} f_i(\mathbf{x}) = \sum_{\mathbf{a} \in \partial_{\mathbf{v}} A_i} c_{i\mathbf{a}} \mathbf{x}^{\mathbf{a}}.$$

Bernshteĭn's Second Theorem

The polynomials $f = (f_1, f_2, \ldots, f_n)$ of a system $f(\mathbf{x}) = 0$

- are supported by $\mathcal{A} = (A_1, A_2, \ldots, A_n)$; and
- have Newton polytopes $\mathcal{P} = (P_1, P_2, \ldots, P_n)$.

For $\mathbf{v} \neq \mathbf{0}$, initial forms $\mathrm{in}_{\mathbf{v}} f = (\mathrm{in}_{\mathbf{v}} f_1, \mathrm{in}_{\mathbf{v}} f_2, \ldots, \mathrm{in}_{\mathbf{v}} f_n)$

- are supported by $\partial_{\mathbf{v}} \mathcal{A} = (\partial_{\mathbf{v}} A_1, \partial_{\mathbf{v}} A_2, \ldots, \partial_{\mathbf{v}} A_n)$; and
- have Newton polytopes $\partial_{\mathbf{v}} \mathcal{P} = (\partial_{\mathbf{v}} P_1, \partial_{\mathbf{v}} P_2, \ldots, \partial_{\mathbf{v}} P_n)$,

We denote the mixed volume of $\mathcal{P}$ by $V(\mathcal{P})$, $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$.

Theorem (Bernshteĭn's theorem B)

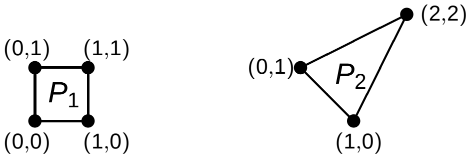
If for all $\mathbf{v} \neq \mathbf{0}$ such that $\mathrm{in}_{\mathbf{v}} f(\mathbf{x}) = \mathbf{0}$ has no solutions in $(\mathbb{C}^*)^n$, then $V(\mathcal{P})$ is exact and all solutions are isolated. Otherwise, for $V(\mathcal{P}) \neq 0$: $V(\mathcal{P}) >$ #isolated solutions.

general position

The system

$$f(\mathbf{x}) = \begin{cases} c_{1,(1,1)}x_1x_2 + c_{1,(1,0)}x_1 + c_{1,(0,1)}x_2 + c_{1,(0,0)} = 0 \\ c_{2,(2,2)}x_1^2x_2^2 + c_{2,(1,0)}x_1 + c_{2,(0,1)}x_2 = 0. \end{cases}$$

has Newton polygons:



$\forall \mathbf{v} \neq \mathbf{0} : \partial_{\mathbf{v}} A_1 + \partial_{\mathbf{v}} A_2 \leq 3 \Rightarrow V(P_1, P_2) = 4$ is always exact,

for all nonzero coefficients of f, because ≥ 4 monomials are needed for $\mathrm{in}_{\mathbf{v}} f(\mathbf{x}) = \mathbf{0}$ to have all its roots in $(\mathbb{C}^*)^2$.

Bernhteǐn's Second Theorem

Puiseux series

Consider the solution paths in a homotopy going from a generic to a specific polynomial system.

Theorem

$\forall \mathbf{x}(t)$, $h(\mathbf{x}(t), t) = (1-t)g(\mathbf{x}(t)) + t\, f(\mathbf{x}(t)) = \mathbf{0}$,
$\exists s > 0$, $m \in \mathbb{N} \setminus \{0\}$, $\mathbf{v} \in \mathbb{Z}^n$:

$$\left\{ \begin{array}{ll} x_i(s) = b_i s^{\mathbf{v}_i}(1 + O(s)), & i = 1, 2, \ldots, n, \\ t(s) = 1 - s^m & \text{for } t \approx 1, s \approx 0. \end{array} \right.$$

The number m is called the *winding number* of the solution at the end of the path ($m \leq$ the multiplicity).

The winding number is the smallest number so that $\mathbf{z}(2\pi m) = \mathbf{z}(0)$, with $\mathbf{z}(\theta)$ a solution path of $h(\mathbf{z}(\theta), t(\theta)) = \mathbf{0}$, winding around 1 with values for the continuation parameter t defined by $t = 1 + (t_0 - 1)e^{i\theta}$, as $t_0 \approx 1$.

diverging paths

$$\forall \mathbf{x}(t), h(\mathbf{x}(t), t) = (1-t)g(\mathbf{x}(t)) + t\, f(\mathbf{x}(t)) = \mathbf{0},$$
$$\exists s > 0, m \in \mathbb{N} \setminus \{0\}, \mathbf{v} \in \mathbb{Z}^n:$$
$$\left\{ \begin{array}{ll} x_i(s) = b_i s^{\mathbf{v}_i}(1 + O(s)), & i = 1,2,\ldots,n, \\ t(s) = 1 - s^m & \text{for } t \approx 1, s \approx 0. \end{array} \right.$$

At the end of a path, when does $\lim\limits_{t \rightarrow 1} x_i(t) \in \mathbb{C}^*$?

We can characterize the divergence of the path $\mathbf{x}(t)$ by the leading exponents $\mathbf{v}$ in the power series

$$x_i(t) \left\{ \begin{array}{l} \rightarrow \infty \\ \in \mathbb{C}^* \\ \rightarrow 0 \end{array} \right. \quad \Leftrightarrow \quad \mathbf{v}_i \left\{ \begin{array}{l} < 0 \\ = 0 \\ > 0 \end{array} \right.$$

A solution at ∞ and a solution with zero components are regarded (or disregarded) equally.

initial forms

We assume $\lim_{t \to 1} x_i(t) \notin \mathbb{C}^*$, and $\mathbf{v}_i \neq 0$.

Substituting $x_i(s) = b_i s^{\mathbf{v}_i}(1 + O(s))$, $i = 1, 2, \ldots, n$,
$t(s) = 1 - s^m, s \approx 0$ into $h(\mathbf{x}, t) = (1-t)g(\mathbf{x}) + t\, f(\mathbf{x}) = \mathbf{0}$:

$$h(\mathbf{x}(s), t(s)) = \underbrace{f(\mathbf{x}(s))}_{\text{dominant as } s \to 0} + s^m(g(\mathbf{x}(s)) - f(\mathbf{x}(s))) = \mathbf{0}.$$

As $s \to 0$, the choice of g does not matter.

$$f_i(\mathbf{x}) = \sum_{\mathbf{a} \in A_i} c_{i\mathbf{a}} \mathbf{x}^{\mathbf{a}} \rightarrow f_i(\mathbf{x}(s)) = \underbrace{\sum_{\mathbf{a} \in A_i} c_{i\mathbf{a}} \prod_{i=1}^{n} b_i^{a_i} s^{\langle \mathbf{a}, \mathbf{v} \rangle}}_{\text{in}_{\mathbf{v}} f_i(\mathbf{x}(s)) \text{ dominant}} (1 + O(s)).$$

Monomials in $\text{in}_{\mathbf{v}} f$ dominate as $s \to 0$ as they have exponents whose inner product is minimal with $\mathbf{v}$.
Moreover, we have $\text{in}_{\mathbf{v}} f_i(\mathbf{b}) = 0$, for some $\mathbf{b} \in (\mathbb{C}^*)^n$.

Bernhteǐn's Second Theorem

logarithms of paths

For $s \rightarrow 0$, the power series for a solution path $\mathbf{x}(s)$ is

$$x_i(s) = b_i s^{v_i/m}(1 + c_i s^{1/m} + O(s^{2/m})), \quad i = 1, 2, \ldots, n.$$

For a diverging path, b_i is not of prime interest, we want

- to find the direction $\mathbf{v}$ for $\partial_{\mathbf{v}}\mathcal{P}$ and $\text{in}_{\mathbf{v}} f$; and
- to approximate the winding number m *first*.

Because we want the powers of s, we take logarithms:

$$\log(|x_i(s)|) = \log(|b_i|) + \frac{v_i}{m}\log(s) + \log(|1 + c_i s^{1/m} + O(s^{2/m})|).$$

The Taylor series for $\log(1 + x) = x + O(x^2)$, so we use

$$\log(|x_i(s)|) \approx \log(|b_i|) + \frac{v_i}{m}\log(s) + |c_i| s^{1/m}, \quad i = 1, 2, \ldots, n.$$

geometric step size

As we get closer to our target system we have to decrease our step size when dealing with a difficult path.

For the purpose of extrapolation, we better decrease the step size geometrically, i.e., for some λ, $0 < \lambda < 1$, consecutive values $t_0, t_1, \ldots, t_k$ of t satisfy

$$1 - t_k = \lambda(1 - t_k) = \cdots = \lambda^k(1 - t_0)$$

and for the corresponding s-values we have

$$s_k = \lambda^{1/m} s_{k-1} = \cdots = \lambda^{k/m} s_0.$$

geometric sampling

Starting at $s_0 \approx 0$, we sample at $s_1 = \lambda s_0$, $s_2 = \lambda^2 s_0$

$$\begin{aligned}
\log(|x_i(s_0)|) &\approx \log(|b_i|) + \frac{v_i}{m}\log(s_0) + |c_i| s_0^{1/m}, \\
\log(|x_i(s_1)|) &\approx \log(|b_i|) + \frac{v_i}{m}\log(\lambda s_0) + |c_i| (\lambda s_0)^{1/m}, \\
\log(|x_i(s_2)|) &\approx \log(|b_i|) + \frac{v_i}{m}\log(\lambda^2 s_0) + |c_i| (\lambda^2 s_0)^{1/m}.
\end{aligned}$$

Observe we have a linear system in v_i/m, a first-order approximation for v_i is $v_{kk+1} := \log|x_i(s_{k+1})| - \log|x_i(s_k)|$, with the general extrapolation formula in $v_{k..\ell}$:

$$v_{k..\ell} = v_{k..\ell-1} + \frac{v_{k+1..\ell} - v_{k..\ell-1}}{1-\lambda}$$

which results in $v_i = m\dfrac{v_{0..r}}{\log(\lambda)} + O(s_0^r)$.

extrapolating for m

The formula for $v_{k..\ell}$ assumes the winding number m. If we examine the expansion of the errors:

$$\begin{aligned} e_i^{(k)} &= (\log|x_i(s_k)| - \log|x_i(s_{k+1})|) \\ &\quad -(\log|x_i(s_{k+1})| - \log|x_i(s_{k+2})|) \\ &= c_1 \lambda^{k/m} s_0 (1 + O(\lambda^{k/m})), \end{aligned}$$

we find similar extrapolation formulas to approximate m: $e_i^{(kk+1)} := \log(e_i^{(k+1)}) - \log(e_i^{(k)})$,

$$e_i^{(k..\ell)} = e_i^{(k+1..\ell)} + \frac{e_i^{(k..\ell-1)} - e_i^{(k+1..\ell)}}{1 - \lambda_{k..\ell}}$$

with $\lambda_{k..\ell} = \lambda^{(\ell-k-1)/m_{k..\ell}}$.

So we obtain $m_{k..\ell} = \dfrac{\log(\lambda)}{e_i^{(k..\ell)}} + O(\lambda^{(\ell-k)k/m})$.

Summary + Exercises

Every facet of a Newton polytope corresponds to a plane at ∞. Initial forms are supported on faces of Newton polytopes and their solutions are solutions at ∞.

Exercises:

1. Verify that the triangulation on the first slide is regular, i.e.: assign heights to the points so that the simplices of the triangulation are the projections of facets on the lower hull of the lifted polytope.
   How many other regular triangulations can you find?

more exercises

2. We can define a multiprojective weighted transformation for the system on the first slide, taking into account the two inner normals $(-2,+1)$ and $(+1,-2)$ to the hyperplanes at infinity, using the respective extra coordinates z_{01} and z_{02}. Apply the substitution $x_1 = z_{01}^{-2} z_{02}^{+1} z_1$ and $x_2 = z_{01}^{+1} z_{02}^{-2} z_2$ to the system on the first slide. Examine the solutions for $(z_{01} = 0, z_{02} = 1)$ and for $(z_{01} = 1, z_{02} = 0)$.
3. For the system in the format with a graph use the first formulation to find the incidence matrices I_a and I_K.

three more exercises

4. Verify that the mixed volume of the system with polygons in general position is indeed four.
5. Consider the homotopy $h(x,t) = x^2 - 1 + 2t - t^2 = 0$ for t going from 0 to 1. Justify the following statement: Although $h(x,t) = 0$ has a double root at $t = 1$, the winding number equals one.
6. Consider $x(s) = bs^{v/m}(1 + cs^{1/m})$, for $v = 1, 2$ and $m = 2, 3$, taking random values for b and c. Apply geometric sampling of $x(s)$ at values for s close enough to 0 to recover the values for v and m.