Bernshteĭn's second theorem

We consider a generalization of Kushnirenko's theorem, due to Bernshteĭn [1]. Our presentation copies part of [5]. Bernshteĭn's second theorem was known in some form to chemists, so it is fitting that our application comes from chemistry [2].

1 Solutions at Infinity

Consider the following polynomial system:

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

If we subtract the equations from each other we obtain $x_1 x_2 + 1 = 0$. Substituting then $x_2 = 1/x_1$ into the first equation and multiplying by x_1 leads to a quadric. So the system has two solutions.

Since the polynomials in $f(\mathbf{x}) = \mathbf{0}$ share the same support, Kushnirenko's theorem applies, see Figure 1.

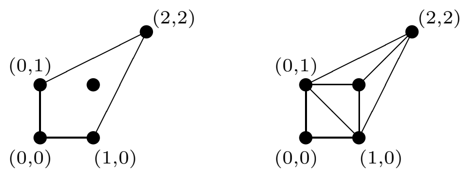

Figure 1: The Newton polygon P spanned by $A = \{(2,2),(1,1),(1,0),(0,1),(0,0)\}$ and a triangulation of P.

Recall that the unit triangle has unit area, from the triangulation in Figure 1 and Kushnirenko's theorem we may expect 4 solutions. So, there should be two solutions at infinity. To compute the solutions at infinity 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

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

Solutions at infinity are solutions with $z_0 = 0$ and not all other coordinates equal to zero. 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 an unsatisfactory result, as we expected to find two, not four solutions at infinity.

The projective transformation defined by $x_1 = z_1 z_0^{-1}$ and $x_2 = z_2 z_0^{-1}$ assumes one hyperplane at infinity, defined by $z_0 = 0$. The exponents of z_0 in this transformation -1 and -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:

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

Setting $z_0 = 0$ now leaves us with $z_1^2 z_2^2 + z_1 = 0$. Accounting for the solution at infinity in a polyhedral way happens by consideration of the monomial closest to the edge that supports $z_1^2 z_2^2 + z_1 = 0$, i.e.: $z_1 z_2$, and adding as second equation $z_1 z_2 - z_1 = 0$. Because we want a solution in $(\mathbb{C}^*)^2$ we may divide by z_1 and solve $z_1 z_2^2 + 1 = 0 = z_2 - 1$ to find $[0 : -1 : +1]$ as solution at infinity. The other solution at infinity is found by considering the projective transformation defined by the other 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.

2 Mass Action Kinetics

The equations to compute the steady states of an oxidation of H_2 on a catalytic surface [2] yield the system

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

where the variables x_1, x_2, x_3, and x_4 are the concentrations of O, H, H_2O, and H_2O_f respectively; and x_5 is the amount of free space on the surface. The parameters $k_{i,j}$ are the so-called rate constants, they are real positive numbers. One conservation law must be added, given by a linear equation:

$$2x_1 + x_2 + 2x_3 + 2x_4 + 2x_5 - c_1 = 0. \quad (5)$$

In matrix form, the system (4) becomes

$$\begin{bmatrix} -1 & 0 & 0 & 0 & 0 & 0 & -2 & 2 & 0 \\ -2 & -2 & 2 & 0 & 0 & 0 & 0 & 0 & -2 \\ 1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & -2 & 0 & 0 & -2 \\ 1 & 1 & -1 & 1 & 0 & 2 & 2 & -2 & 3 \end{bmatrix} \begin{bmatrix} k_{2,1} & x_1x_2^2 \\ k_{9,3} & x_2^2 \\ k_{3,9} & x_5 \\ k_{9,4} & x_3 \\ k_{5,4} & x_3 \\ k_{10,6} & x_4^2 \\ k_{10,7} & x_1^2 \\ k_{7,10} & x_5^2 \\ k_{11,8} & x_2x_4 \end{bmatrix} = \mathbf{0}. \quad (6)$$

The drawbacks of this matrix form are that some columns in the coefficient matrix are the same, except for their sign, and that some monomials appear twice with different constants.

In [2], using a directed weighted bipartite graph between complexes, the system in (4) and (5) becomes

$$f(\mathbf{x}) = \begin{cases} Y_s I_a I_K \Psi(\mathbf{x}) = \mathbf{0} \\ 2x_1 + x_2 + 2x_3 + 2x_4 + 2x_5 - c_1 = 0. \end{cases} \quad (7)$$

where Y_s is a fixed matrix of integer coefficients, the matrices I_a and I_K are incidence matrices derived from the graph, and $\Psi(\mathbf{x})$ is a vector of monomials. For the system in (4), the data are

$$Y_s = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 & 0 \\ 2 & 0 & 2 & 0 & 0 & 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 2 & 3 \end{bmatrix} \quad (8)$$

and

$$\Psi(\mathbf{x}) = \left(x_1x_2^2, x_3x_5, x_2^2, x_3, x_4, x_4^2, x_1^2, x_2x_4, x_5, x_5^2, x_5^3\right)^T. \quad (9)$$

The number of monomials in $\Psi(\mathbf{x})$ equals the number of complexes. For monomials in $\Psi(\mathbf{x})$ which do not appear in the original system, the corresponding column in I_K is zero. The system in (7) is in a more convenient format, its study is developed in [2].

3 Bernshteĭn's Second Theorem

When tracing solution paths diverging to infinity, one may wonder when to stop. After all, infinity is pretty far off, and even if good knowledge of the application domain gives us good bounds on the size of the solutions, we do not want to miss valid solutions with large components. If a path seems to diverge, we must know whether we have true divergence or convergence to a root with large components. Bernshteĭn's second theorem [1] will provide us with a certificate of divergence.

For a system $f(\mathbf{x}) = 0$, supported by $\mathcal{A} = (A_1, A_2, \ldots, A_n)$, we write its equations $f = (f_1, f_2, \ldots, f_n)$ as

$$f_i(\mathbf{x}) = \sum_{\mathbf{a} \in A_i} c_{i\mathbf{a}} \mathbf{x}^{\mathbf{a}}, \quad c_{i\mathbf{a}} \in \mathbb{C}^*, \quad \mathbf{x}^{\mathbf{a}} = x_1^{a_1} x_2^{a_2} \cdots x_n^{a_n}, \quad i = 1, 2, \ldots, n. \tag{10}$$

The Newton polytopes of f are denoted by $\mathcal{P} = (P_1, P_2, \ldots, P_n)$, with $P_i := \mathrm{conv}(A_i)$, $i = 1, 2, \ldots, n$. Then for any $\mathbf{v} \neq \mathbf{0}$, we define the tuple of faces $\partial_{\mathbf{v}} \mathcal{P} = (\partial_{\mathbf{v}} P_1, \partial_{\mathbf{v}} P_2, \ldots, \partial_{\mathbf{v}} P_n)$, as $\partial_{\mathbf{v}} P_i := \mathrm{conv}(\partial_{\mathbf{v}} A_i)$, with

$$\partial_{\mathbf{v}} A_i := \{ \ \mathbf{a} \in A_i \mid \langle \mathbf{a}, \mathbf{v} \rangle = \min_{\mathbf{a}' \in A_i} \langle \mathbf{a}', \mathbf{v} \rangle \ \}. \tag{11}$$

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

$$\mathrm{in}_{\mathbf{v}} f_i(\mathbf{x}) = \sum_{\mathbf{a} \in \partial_{\mathbf{v}} A_i} c_{i\mathbf{a}} \mathbf{x}^{\mathbf{a}}. \tag{12}$$

We write $\mathrm{in}_{\mathbf{v}} f = (\mathrm{in}_{\mathbf{v}} f_1, \mathrm{in}_{\mathbf{v}} f_2, \ldots, \mathrm{in}_{\mathbf{v}} f_n)$ as the initial form of the system f determined by $\mathbf{v} \neq \mathbf{0}$. The mixed volume of $\mathcal{P}$ is denoted by $V(\mathcal{P})$ and $\mathbb{C}^* = \mathbb{C} \setminus \{0\}$.

Theorem 3.1 (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.*

Interestingly, the Newton polytopes may often be in general position, i.e.: $V(\mathcal{P})$ is exact for every nonzero choice of the coefficients. Consider for example the following system:

$$f(\mathbf{x}) = \left\{ \begin{array}{r} c_{1,(1,1)} x_1 x_2 + c_{1,(1,0)} x_1 + c_{1,(0,1)} x_2 + c_{1,(0,0)} = 0 \\ c_{2,(2,2)} x_1^2 x_2^2 + c_{2,(1,0)} x_1 + c_{2,(0,1)} x_2 = 0. \end{array} \right. \tag{13}$$

We show the tuple of Newton polytopes in Figure 2.

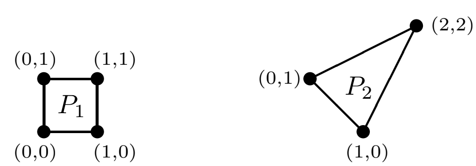

Figure 2: Two Newton polygons in general position: $\forall \mathbf{v} \neq \mathbf{0} : \partial_{\mathbf{v}} A_1 + \partial_{\mathbf{v}} A_2 \leq 3 \Rightarrow V(P_1, P_2) = 4$ is always exact, for all nonzero choices of the coefficients of f, because we need at least four monomials for $\partial_{\mathbf{v}} f(\mathbf{x}) = \mathbf{0}$ to have all its roots in $(\mathbb{C}^*)^2$.

While the observation in Figure 2 would let us believe that the mixed volume always provides a sharp root count, we have to keep in mind that the vertices of the polytopes are not randomly chosen. The vertices occur as the exponents in the polynomials. For instance, general Newton polytopes are almost never simplicial, we usually find k-dimensional faces spanned by far more than $k + 1$ vertices.

4 Puiseux Series and Initial Forms

Following Bernshteĭn we look at what happens when we consider the solution paths in a homotopy going from a generic to a specific polynomial system. At the limit of the paths, we look at the power series expansion, using the following result.

Theorem 4.1 *$\forall \mathbf{x}(t)$, $h(\mathbf{x}(t), t) = (1-t)g(\mathbf{x}(t)) + tf(\mathbf{x}(t)) = \mathbf{0}$,*
$\exists s > 0$, $m \in \mathbb{N} \setminus \{0\}$, $\mathbf{v} \in \mathbb{Z}^n$: $\begin{cases} x_i(s) = b_i s^{\mathbf{v}_i}(1 + O(s)), & i = 1, 2, \ldots, n, \\ t(s) = 1 - s^m & \text{for } t \approx 1, s \approx 0. \end{cases}$

The number m is called the *winding number* of the solution at the end of the path (not to be confused with the multiplicity). The winding number is the smallest number so that $\mathbf{z}(2\pi m) = \mathbf{z}(0)$, if we consider $\mathbf{z}(\theta)$ 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 $t_0 \approx 1$.

At the end of a path, when does $\lim_{t \to 1} x_i(t) \in \mathbb{C}^*$? From Theorem 4.1, we can characterize the divergence of the path $\mathbf{x}(t)$ by the leading exponents $\mathbf{v}$ in the power series:

$$x_i(t) \begin{cases} \to \infty \\ \in \mathbb{C}^* \\ \to 0 \end{cases} \quad \Leftrightarrow \quad \mathbf{v}_i \begin{cases} < 0 \\ = 0 \\ > 0 \end{cases} \tag{14}$$

From this simple observation we see that a solution at infinity and a solution with zero components are regarded (or disregarded) equally.

Next we show the relation between face systems and power series. Assuming $\lim_{t \to 1} x_i(t) \not\in \mathbb{C}^*$, and $\mathbf{v}_i \neq 0$, we consider a diverging path.

First we substitute the power series $x_i(s) = b_i s^{\mathbf{v}_i}(1 + O(s))$, $i = 1, 2, \ldots, n$, $t(s) = 1 - s^m, s \approx 0$ into the homotopy $h(\mathbf{x}, t) = (1-t)g(\mathbf{x}) + tf(\mathbf{x}) = \mathbf{0}$. We find

$$h(\mathbf{x}(s), t(s)) = \underbrace{f(\mathbf{x}(s))}_{\text{dominant as } s \to 0} + s^m(g(\mathbf{x}(s)) - f(\mathbf{x}(s))) = \mathbf{0}. \tag{15}$$

Thus (as expected), the choice of the start system $g(\mathbf{x}) = \mathbf{0}$ plays no role in what happens as s approaches zero. Let us now see what the substitution does to the ith polynomial:

$$f_i(\mathbf{x}) = \sum_{\mathbf{a} \in A_i} c_{i\mathbf{a}} \mathbf{x}^{\mathbf{a}} \to f_i(\mathbf{x}(s)) = \underbrace{\sum_{\mathbf{a} \in A_i} c_{i\mathbf{a}} \prod_{i=1}^{n} b_i^{a_i} s^{\langle \mathbf{a}, \mathbf{v} \rangle}}_{\text{in}_{\mathbf{v}} f_i(\mathbf{x}(s)) \text{ dominant}} (1 + O(s)). \tag{16}$$

Arranging the monomials in $f(\mathbf{x}(s))$ in increasing order of powers of s, we see that the monomials that become dominant as $s \to 0$ have exponents whose inner product is minimal with $\mathbf{v}$. Recall that we characterize these exponents by the face of the support A_i in the direction of $\mathbf{v}$, see (11). Moreover, as $f_i(\mathbf{x}(s)) = 0$ for $s \to 0$, we see from the result of the substitution that then $\text{in}_{\mathbf{v}} f_i(\mathbf{b}) = 0$, and thus $\text{in}_{\mathbf{v}} f(\mathbf{b}) = \mathbf{0}$ for some $\mathbf{b} \in (\mathbb{C}^*)^n$.

This is the key idea in the proof of Bernshteĭn's second theorem. Like his first theorem, his idea is very constructive: follow the direction of a diverging path and (in addition to a solution at infinity) we find an initial form system which has solutions in $(\mathbb{C}^*)^n$. This initial form system forms a certificate for the mixed volume to overshoot the actual number of roots.

The application of numerical extrapolation techniques is most appropriate to compute this certificate.

5 Richardson Extrapolation

With Richardson extrapolation on the logarithms of the solution components we find the leading powers of the Puiseux series expansions. A closer inspection of the errors of the error expansion reveals that a similar extrapolation scheme can be applied to approximate the winding number m.

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 the continuation parameter t satisfy $1 - t_k = \lambda(1 - t_k) = \cdots = \lambda^k(1 - t_0)$ and for the corresponding sequence of s-values we have $s_k = \lambda^{1/m} s_{k-1} = \cdots = \lambda^{k/m} s_0$.

For s approaching 0, the power series for a solution path $\mathbf{x}(s)$ has the following form:

$$x_i(s) = b_i s^{v_i/m}(1 + c_i s^{1/m} + O(s^{2/m})), \quad i = 1, 2, \ldots, n. \tag{17}$$

Because we are interested in the powers of s, we take logarithms of the magnitudes of the points sampled along the path, for $i = 1, 2, \ldots, n$:

$$\log(|x_i(s)|) = \log(|b_i|) + \frac{v_i}{m}\log(s) + \log(|1 + c_i s^{1/m} + O(s^{2/m})|). \tag{18}$$

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

$$\log(|x_i(s)|) \approx \log(|b_i|) + \frac{v_i}{m}\log(s) + |c_i| s^{1/m}, \quad i = 1, 2, \ldots, n. \tag{19}$$

Starting at some $s_0 \approx 0$, we apply geometric sampling $s_1 = \lambda s_0$, $s_2 = \lambda^2 s_0$ and consider, for $i = 1, 2, \ldots, n$:

$$\log(|x_i(s_0)|) \approx \log(|b_i|) + \frac{v_i}{m}\log(s_0) + |c_i| s_0^{1/m}, \tag{20}$$

$$\log(|x_i(s_1)|) \approx \log(|b_i|) + \frac{v_i}{m}\log(\lambda s_0) + |c_i|(\lambda s_0)^{1/m}, \tag{21}$$

$$\log(|x_i(s_2)|) \approx \log(|b_i|) + \frac{v_i}{m}\log(\lambda^2 s_0) + |c_i|(\lambda^2 s_0)^{1/m}. \tag{22}$$

Via elimination on the linear equations above, a first-order approximation for v_i is given by v_{kk+1} with the general extrapolation formula in $v_{k..l}$:

$$v_{kk+1} := \log|x_i(s_{k+1})| - \log|x_i(s_k)|, \quad v_{k..l} = v_{k..l-1} + \frac{v_{k+1..l} - v_{k..l-1}}{1 - \lambda} \tag{23}$$

which results in $v_i = m\frac{v_{0..r}}{\log(\lambda)} + O(s_0^r)$. While we can make the order r of the extrapolation as high as we like (thereby increasing the accuracy of v_i). Observe that the formula assumes we know the winding number m.

If we examine the expansion of the errors:

$$e_i^{(k)} = (\log|x_i(s_k)| - \log|x_i(s_{k+1})|) \tag{24}$$

$$-(\log|x_i(s_{k+1})| - \log|x_i(s_{k+2})|) \tag{25}$$

$$= c_1 \lambda^{k/m} s_0 (1 + 0(\lambda^{k/m})), \tag{26}$$

we find similar extrapolation formulas to approximate m:

$$e_i^{(kk+1)} := \log(e_i^{(k+1)}) - \log(e_i^{(k)}), \quad e_i^{(k..l)} = e_i^{(k+1..l)} + \frac{e_i^{(k..l-1)} - e_i^{(k+1..l)}}{1 - \lambda_{k..l}} \tag{27}$$

with $\lambda_{k..l} = \lambda^{(l-k-1)/m_{k..l}}$. So we obtain $m_{k..l} = \frac{\log(\lambda)}{e_i^{(k..l)}} + O(\lambda^{(l-k)k/m})$.

These formulas are applied in polyhedral endgames [3]. Numerically, as $s \to 0$, the solution may become more and more singular up to the point where extrapolation no longer give good results because of accumulated roundoff, so we cannot take s too small. However, s has to be small enough to observe the divergence of the solution path. This tradeoff consideration leads to *the endgame operation range* [4]. With multiprecision arithmetic we can ensure that this range is not empty.

6 Exercises

1. Verify that the triangulation in (1) 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?

2. We can define a multiprojective weighted transformation for the system in (1), 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 in (1). 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 (7), use (4) to find the incidence matrices I_a and I_K.

4. Verify that the mixed volume of the system in (13) 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.

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