Introduction to Gröbner Bases with Applications to the Geometry of Value Functions

Ryan A. Anderson

Department of Statistics and Data Science
University of California, Los Angeles

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Monomial Ideals and Leading Terms

- Want to be able to move from ideals in a polynomial ring to ideals generated by a finite set of monomials - these are *monomial ideals*
- The natural thing to do is to fix a monomial order on the ideal I and take the ideal generated by the leading term of every polynomial in the ideal, $\langle LT(I) \rangle$
  - e.g. A lexicographic ordering on the polynomial ring $K[x, y, z]$ with $x > y > z$ implies $x^2 > y^2, x^2 > xz$, etc.
- This may be unworkable - we would rather take only the leading terms of the generators of $I = \langle f_1, \ldots, f_n \rangle$. But $\langle LT(I) \rangle$ does not always equal $\langle LT(f_1), \ldots LT(f_s) \rangle$!

Take $I = \langle f_1, f_2 \rangle = \langle x^2 + 2xy^2, xy + 2y^3 - 1 \rangle$. $x = x * f_2 - y * f_1$, so $x \in I$. $LT(x) = x \in I$, but think about $\langle LT(f_1), LT(f_2) \rangle = \langle x^2, xy \rangle$. $x \notin \langle x^2, xy \rangle$!

Gröbner Bases and Ideal Membership

- So we need to find a generating set of polynomials $g_1, \dots g_m$ such that for a given ideal I, $\langle LT(I) \rangle = \langle LT(g_1), \dots LT(g_m) \rangle$
  - The justification for this is Hilbert's basis theorem, which says every ideal in R is finitely generated!
- Now fix a monomial order and consider an ideal I. A finite subset $G = \{g_1, \dots g_m\}$ is a *Gröbner basis* for I if $\langle LT(I) \rangle = \langle LT(g_1), \dots LT(g_m) \rangle$
- The immediate and extremely useful corollary is the following: let G be a Gröbner basis for an ideal $I \subset R$. Then $f \in I \iff$ the remainder after division of f by G is zero, where we divide f by G by finding a linear combination of the generators such that

$$f = e_1 g_1 + \dots e_m g_m + r$$

Buchberger's Algorithm

- Thinking about the relationship between ideal membership and Gröbner bases leads nicely to a method for constructing them: Buchberger's Algorithm
- Let the *S-polynomial* of $f, g \in R$ is

$$S(f,g) = \frac{LCM(LT(f), LT(g))}{LT(f)} f - \frac{LCM(LT(f), LT(g))}{LT(g)} g$$

- Buchberger's Criterion says a subset $G = \{g_1, \dots g_m\}$ of an ideal is a Gröbner basis iff $S(g_m, g_n)$ has a remainder of zero after division by G
- Buchberger's Algorithm then allows us to construct a Gröbner basis by adding any non-zero remainders of $S(g_m . g_n)$ to the subset

Using Buchberger's Algorithm

Consider $G = \langle xy - x, x^2 - y \rangle$. Fix the *graded lexicographic order* and $x > y$. We want to see if this is a Gröbner basis, or if not, find one

$$LT(f_1) = xy, LT(f_2) = x^2, LCM(LT(f_1), LT(f_2)) = x^2y$$

$$S(f_1, f_2) = \frac{x^2y}{xy}(xy - x) - \frac{x^2y}{x^2}(x^2 - y) = -x^2 + y^2$$

$$S(f_1, f_2) = -f_2 + (y^2 + y)$$

$$\text{Let } G' = \langle xy - x, x^2 - y, y^2 + y \rangle. \text{ Then } S(f_1, f_2) = -f_2 + f_3$$

$$S(f_1, f_3) = \frac{xy^2}{xy}(xy - x) - \frac{xy^2}{y^2}(y^2 + y) = 0$$

$$S(f_2, f_3) = \frac{x^2y^2}{x^2}(x^2 - y) - \frac{x^2y^2}{y^2}(y^2 + y) = -2y^3 \Rightarrow f_3$$

Then $G' = \langle xy - x, x^2 - y, y^2 + y \rangle$ is a Gröbner basis.

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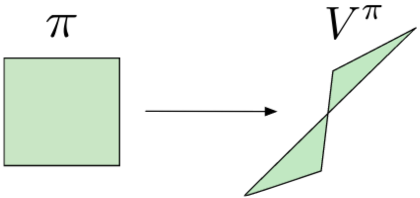
The Value Function in Reinforcement Learning

- In a reinforcement learning setting, we are interested in an MDP $\langle S, A, R, P, \gamma \rangle$. For a given policy $\pi : S \to \mathbb{P}(A)$, the Bellman equation for the value function gives us

$$(I - \gamma P^{\pi})V^{\pi} = r^{\pi}$$

- The policies π always live in the unit box and take the form

$$\pi = \begin{bmatrix} p_1 & p_2 \\ 1 - p_1 & 1 - p_2 \end{bmatrix}$$



Solution Sets of Interval Matrix Equations

- Because of the box constraints on our policies, we can reinterpret the Bellman equation as an *interval matrix equation* of the form $A(p)x = b(p)$
- Solutions to interval matrix equations have been studied for a very long time! In particular a result of [4] gives the following:

Consider for an interval matrix equation $A(p)x = b(p)$, the parametric solution set $\Sigma^p = \{x \in \mathbb{R}^n | \exists p \in [p], A(p)x = b(p)\}$.

- Let $K = \{1, \dots, k\}$ and consider $Q(n-1, k)$ the set of all subsets of K containing $n-1$ elements. For a vector $p \in \mathbb{R}^k$ and $q \in Q(n-1, k)$ define $q* = K/q$ and $p_q = (p_i)_{i \in q}$ and $p_{q*} = (p_i)_{i \in q*}$.
- If $A(p)$ is nonsingular for all $p \in [p]$ and $k \leq n$, then

$$\partial \Sigma^p = \cup_{q \in Q(n-1,k)} \{x(p_q, p_{q*}^-)|_{p_q \in [p_q]}, x(p_q, p_{q*}^+)|_{p_q \in [p_q]}\}$$

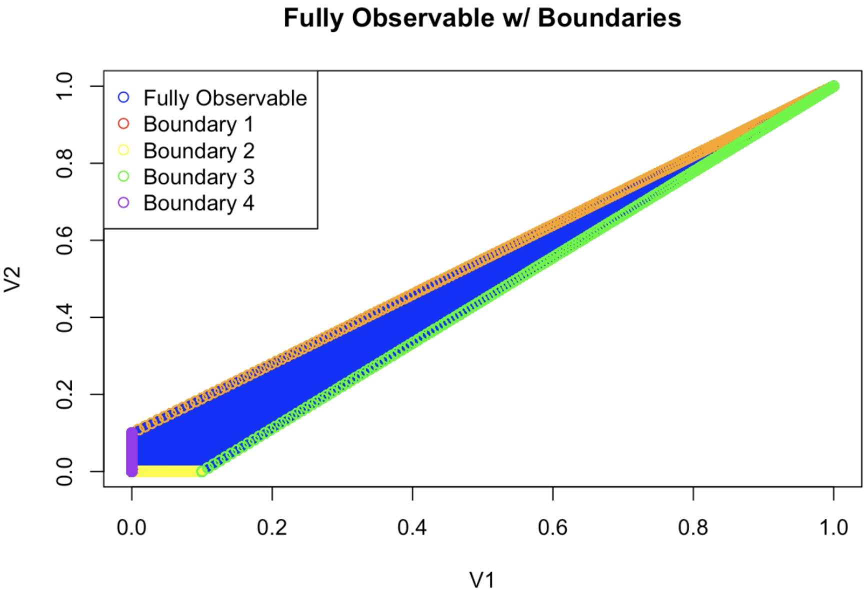
Solution Sets of the Bellman Equation

- Upshot of Popova's theorem is a very cool result – the boundaries of the polytope (or the image under $A(p)$) are given by images of the boundaries of the parameter!
- We can also use Popova's theorem to calculate the boundaries of the value function polytope! All we need is that $A(p) = I - \gamma P^{\pi}$ is invertible over the parametric domain, which we get from a result in [2]
- In particular, for a fully observable MDP with basically unit hyperparameters, we get

$$V^{\pi}(p_1, 0) = \begin{bmatrix} 0 \\ 1 - p_1 \end{bmatrix}, V^{\pi}(p_1, 1) = \begin{bmatrix} -\frac{p_1 - 2}{p_1} \\ -\frac{2p_1 - 2}{p_1} \end{bmatrix}$$

$$V^{\pi}(0, p_2) = \begin{bmatrix} -\frac{2p_2}{p_2 - 1} \\ -\frac{p_2 + 1}{p_2 - 1} \end{bmatrix}, V^{\pi}(1, p_2) = \begin{bmatrix} p_2 \\ 0 \end{bmatrix}$$

Solution Sets of the Bellman Equation



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Implicitization with Gröbner Bases

- Above, we obtained parametric descriptions of the boundaries of the solution sets, but we're interested the polytope as a purely geometric object, and so would like to find an implicit description
- The benefit of Gröbner bases in our case is *implicitization*, where we use elimination algorithms to get only the variables we care about
  - Gröbner bases are especially good for implicitization because we only need to get rid of the finitely many generators containing the undesirable variables – not usually the case [3]
- The *implicitization algorithm for rational parametrizations* from [1] gives us
  - For an ideal $J = \langle x_1 - \frac{f_1}{g_1}, \dots, x_n - \frac{f_n}{g_n} \rangle$, where $f_i, g_i \in k[t_1, \dots, t_m]$ clear denominators to form the new ideal $J' = \langle x_1 g_1 - f_1, \dots, x_n g_n - f_n, 1 - (\prod g_i) y \rangle$
  - Fix a lexographic monomial order with $y > t_1 > \cdots > t_m > x_1 \cdots > x_n$ and calculate a Gröbner basis for J'
  - The elements of the Gröbner basis not containing $y, t_1, \dots, t_m$ will be the smallest variety containing the parametrization!

Implicitizing the Boundary of the Value Function Polytope

- Let's do the same for the boundary of the VF polytope – we change the hyperparametrization slightly to have $\gamma = 0.9$, giving

$$V_1 = (v_1, v_2 - 1 - p_1), V_2 = (v_1 - \frac{-0.9p_1 + 1.9}{0.81p_1 + 0.19}, v_2 - \frac{-1.9p_1 + 1.9}{0.81p_1 + 0.19})$$
$$V_3 = (v_1 - \frac{-1.9p_2}{0.81p_2 - 1}, v_2 - \frac{-0.9p_2 - 1}{0.81p_2 - 1}), V_4 = (v_1 - p_2, v_2)$$

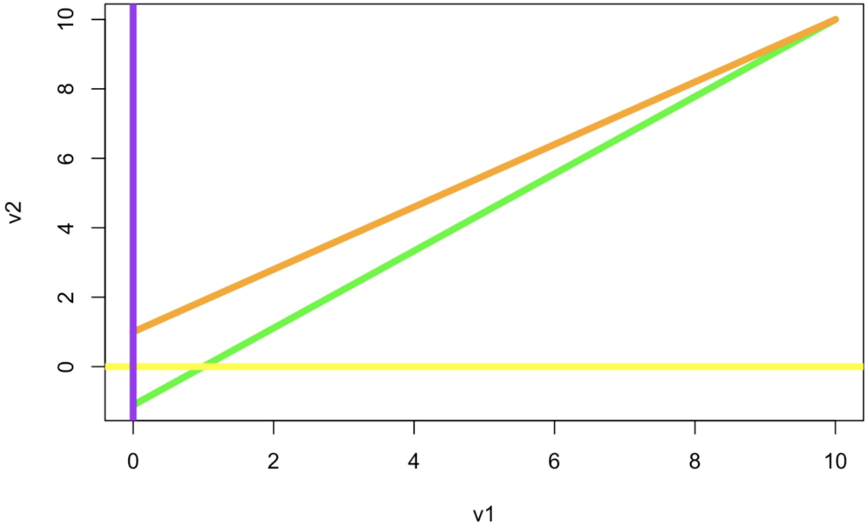
- We only care about boundary pieces 2 and 3, where we clear denominators to get

$$V_2' = \langle (0.81p_1 + 0.19)v_1 - 0.9p_1 + 1.9, (0.81p_1 + 0.19)v_2 - 1.9p_1 + 1.9, 1 - (0.81p_1 + 0.19)y \rangle$$
$$V_3' = \langle (0.81p_1 + 0.19)v_1 - 0.9p_1 + 1.9, (0.81p_1 + 0.19)v_2 - 1.9p_1 + 1.9, 1 - (0.81p_1 + 0.19)y \rangle$$

- Elimination via Gröbner bases then gives

$$V_2' = \langle 10v_1 - 9v_2 - 10 \rangle$$
$$V_3' = \langle 9v_1 - 10v_2 + 10 \rangle$$

Plotting the Solution Set via Implicit Equations



Challenges with Implicitization

- For equations of more than a few terms or indeterminates, implicitization via Gröbner bases can be very slow
  - Moreover, depends on choice of monomial order – we used lex and grlex, but in fact reverse graded lex is fastest
- One other approach: estimating the variety from samples on the curves

References

[1] David A. Cox, John Little, and Donal O'Shea. *Ideals, Varieties, and Algorithms: An Introduction to Computational Algebraic Geometry and Commutative Algebra*. Undergraduate Texts in Mathematics. Springer International Publishing, Cham, 2015.

[2] Robert Dadashi, Adrien Ali Taïga, Nicolas Le Roux, Dale Schuurmans, and Marc G. Bellemare. The Value Function Polytope in Reinforcement Learning, May 2019. arXiv:1901.11524 [cs, stat].

[3] Mateusz Michałek and Bernd Sturmfels. *Invitation to nonlinear algebra*. Number 211 in Graduate studies in mathematics. American Mathematical Society, Providence, Rhode Island, 2021.

[4] E. D. Popova and W. Krämer. Visualizing parametric solution sets. *BIT*, 48(1):95–115, mar 2008.