Toric Geometry of Entropic Regularization

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Abstract

Entropic regularization is a method for large-scale linear programming. Geometrically, one traces intersections of the feasible polytope with scaled toric varieties, starting at the Birch point. We compare this to log-barrier methods, with reciprocal linear spaces, starting at the analytic center. We revisit entropic regularization for unbalanced optimal transport, and we develop the use of optimal conic couplings. We compute the degree of the associated toric variety, and we explore algorithms like iterative scaling.

1 Introduction

Linear programming in standard form is the optimization problem

Minimize
$$c \cdot x$$
 subject to $Ax = b$ and $x > 0$. (1)

Here A is a nonnegative $d \times n$ matrix of rank d with no zero column, $c \in \mathbb{R}^n$ is a row vector, and $b \in \mathbb{R}^d$ is a column vector. This program is feasible if and only if b lies in pos(A), which is the convex polyhedral cone spanned by the columns of A. If c is fixed and generic, and b ranges over pos(A), then the set of optimal bases of (1) defines a regular triangulation of the cone pos(A). This classical result due to Walkup and Wets is explained geometrically in [8, Theorem 1.2.2]. The triangulation is replaced by a continuous shape under a regularization

Minimize
$$c \cdot x + \epsilon \sum_{i=1}^{n} H(x_i)$$
 subject to $Ax = b$ and $x \ge 0$. (2)

Here, H is a strictly convex smooth function on $\mathbb{R}_{\geq 0}$, and ϵ is a positive parameter. For interior point methods, H is taken as a barrier function, meaning that its limit at 0 is $+\infty$. This enables us to remove the constraint $x \geq 0$ in (2). The dual formulation of (2) reads:

Maximize
$$b \cdot p - \epsilon \sum_{i=1}^{n} H^* \left(\frac{1}{\epsilon} \left[A^{\top} p - c \right]_i \right)$$
 over all $p \in \mathbb{R}^d$. (3)

Here, $H^*(s) = \sup_{t \in \mathbb{R}} (st - H(t))$ denotes the Legendre-Fenchel transform of the convex function H, after the latter has been extended to all of \mathbb{R} by setting $H(t) = +\infty$ for t < 0.

The feasible set $P_{A,b} := \{x \in \mathbb{R}^n_{\geq 0} : Ax = b\}$ for (1) is a polytope. For every $\epsilon > 0$, the regularized problem (2) has a unique optimal solution $x^*(\epsilon)$ in the relative interior of $P_{A,b}$, provided the function H is barrier. The curve $\mathcal{C}_{A,b,c} = \{x^*(\epsilon) : 0 \leq \epsilon \leq \infty\}$ connects the distinguished point $x^*(\infty)$ in $P_{A,b}$ to an optimal solution $x^*(0)$ of the linear program (1).

Applying Lagrange multipliers to (2) gives a determinantal representation for $\mathcal{C}_{A,b,c}$:

$$Ax = b$$
 and $\operatorname{rank} \begin{pmatrix} A \\ c \\ H'(x) \end{pmatrix} \le d + 1.$ (4)

The matrix on the right has d+2 rows and n columns. Its last row is the vector of derivatives

$$H'(x) = (H'(x_1), H'(x_2), \dots, H'(x_n)).$$

For generic cost vectors c, the number of independent constraints in (4) equals d+(n-d-1)=n-1, so we expect these to cut out an analytic curve in \mathbb{R}^n . The distinguished interior point $x^*(\infty)$, at which our curve starts, satisfies rank $\binom{A}{H'(x)} \leq d$. For any fixed $\epsilon \in \mathbb{R}_{>0}$, the point $x^*(\epsilon)$ on the curve satisfies rank $\binom{A}{c+\epsilon H'(x)} \leq d$. Moreover, if H and c satisfy certain hypotheses then the curve is algebraic, and we can study its defining ideal in $\mathbb{R}[x_1, x_2, \dots, x_n]$.

We compare two widely used regularizations. The first is the logarithmic barrier function $H(t) = -\log(t)$, where (2) is the standard formulation of an interior point method for (1). This function is self-concordant, which is a key property in convex optimization. The rank condition in (4) translates into polynomials by taking numerators of all maximal minors. These define an algebraic curve $\mathcal{C}_{A,b,c}^{R,+}$ in the polytope $P_{A,b}$. This is known as the central path. Its starting point $x^*(\infty)$ is the analytic center of $P_{A,b}$. The algebraic complexity of these objects are governed by the bounded regions in certain hyperplane arrangements. See [2, 9].

Next consider the entropy function $H(t) = t \cdot \log(t) - t$, whose Legendre-Fenchel transform equals $H^*(s) = \exp(s)$. Here, (2) is the entropic regularization of (1). This approach is popular in machine learning, especially for optimal transport problems [6, 12, 20]. Note that H(t) is strictly convex but not strongly convex. It is not a barrier function since H(t) does not diverge for $t \to 0$. But, its derivative does, and this ensures the minimizer $x^*(\epsilon)$ to be in the relative interior of $P_{A,b}$. To highlight algebraic features, we assume that the cost vector c has integer coordinates. The rank condition in (4) is a system of \mathbb{Z} -linear equations in $\log(x_1), \ldots, \log(x_n)$. These translate into differences of monomials in $\mathbb{R}[x_1, \ldots, x_n]$. Indeed, (4) specifies the toric variety of the integer matrix $\binom{A}{c}$. We obtain the entropic curve $\mathcal{C}_{A,b,c}^T$ by intersecting that toric variety with the linear space $\{Ax = b\}$. Its degree is bounded by the normalized volume of a polytope associated to $\binom{A}{c}$, and $x^*(\infty)$ is the Birch point of $P_{A,b}$.

Example 1 (d = 4, n = 6). We consider the transportation problem of format 2×3 , as in [9, Examples 2 and 14]. We here represent this by a matrix with linearly independent rows:

$$A = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}. \tag{5}$$

To explore the generic behavior for this A, we fix $b = (7, 8, 4, 5)^{\top}$ and c = (1, 0, 1, 0, 2, 5). The transportation polytope $P_{A,b}$ is a hexagon in the affine plane $\{Ax = b\}$ in \mathbb{R}^6 . We use coordinates (x_1, x_2) , as these determine x_3, x_4, x_5, x_6 . First consider its log-barrier geometry. The edges of $P_{A,b}$ specify an arrangement of lines in the plane $\{Ax = b\}$, whose complement has seven bounded regions. Therefore, the analytic center has algebraic degree seven:

$$x^*(\infty) = (1.895889342, 2.337573614, 2.766537044, 2.104110658, 2.662426386, 3.233462956).$$

For generic cost vectors c, the central path has degree five. Two pictures are shown in [9, Figure 1]. For the specific c above, the quintic polynomial defining the central path equals

$$10x_1^4x_2 + 22x_1^3x_2^2 + 8x_1^2x_2^3 - 4x_1x_2^4 - 25x_1^4 - 180x_1^3x_2 - 183x_1^2x_2^2 + \dots + 376x_2^2 + 700x_1 - 280x_2.$$

Now compare this to entropic regularization. The Birch point has rational coordinates:

$$x^*(\infty) = \frac{1}{15}(28, 35, 42, 32, 40, 48) = (1.8666, 2.3333, 2.8000, 2.1333, 2.6666, 3.2000).$$

The rank constraint in (4) translates into the binomial equation $x_1^2 x_3^3 x_5^5 = x_2^5 x_4^2 x_6^3$. The degree drops by one when we intersect with $\{Ax = b\}$. The entropic curve is given by

$$25x_1^5x_2^4 + 85x_1^4x_2^5 + 87x_1^3x_2^6 + 19x_1^2x_2^7 - 8x_1x_2^8 - 250x_1^5x_2^3 - 1275x_1^4x_2^4 + \dots + 1531250x_1^2x_2 - 1071875x_1^2.$$

As the vector c ranges over \mathbb{Z}^6 , the degree of this curve can be arbitrarily large. For non-rational c, the entropic curve is no longer algebraic. This is a general feature of toric geometry.

Note that pos(A) is the cone over a triangular prism, and c determines a triangulation of that prism into three tetrahedra. There are six such triangulations, one for each vertex of $P_{A,b}$. Think of the triangulation as the union of three \mathbb{P}^3 's in \mathbb{P}^5 . Regularization replaces the triangulation by a nearby smooth variety. For the entropic regularization, this is a Segre variety $\mathbb{P}^1 \times \mathbb{P}^2$. For the log-barrier regularization, it is the reciprocal linear space for A. \diamond

The distinction between our two regularizations mirrors that between toric geometry and matroid theory. In statistics, this is the distinction between toric models and linear models [15, Section 1.2]. These objects are central in the study of positive geometries in combinatorics and physics (cf. [19, Section 6]). In Section 2 we develop a comparative theory. After a review of known facts in Proposition 3 and 4, we present our findings in Theorem 6 and 8. They concern the algebraic curves and positive varieties arising from linear programming.

In Section 3 we turn to the optimal transport problem. This is ubiquitous in data science, where entropic regularization is a method of choice [6]. Indeed, in this context the entropy function is preferred over the logarithmic barrier for efficiency reasons. We will come back to this preference in Remark 9. Geometrically, $P_{A,b}$ is a transportation polytope, and Segre varieties regularize triangulations of products of simplices, as seen in Example 1. Our contribution is an extension of this theory to the unbalanced regime, which was studied in [4, 5]. We formulate the discrete conic coupling in eqn. (22), in the spirit of [13].

Section 4 is devoted to the toric geometry and combinatorics of our new variant. The main result is a formula for the algebraic degree of conic optimal transport (Theorem 16). In Section 5 we discuss numerical algorithms for the entropic regularization (2). The task is to compute the points $x^*(\epsilon)$ along the entropic curve $\mathcal{C}_{A,b,c}^T$, and to solve (1) by letting $\epsilon \to 0$.

Remark 2. After completing this paper, we learned that the usage of the term *entropic* barrier varies across the literature. There is a general definition for arbitrary convex bodies, due to Bubeck and Eldan. When restricted to polytopes, this leads to the logarithmic barrier and the analytic center. This connection was developed from the perspective of tropical geometry by Allamigeon et al. in [1]. Their entropic path agrees with the central path, arising from $H(t) = -\log(t)$. What we call the entropic curve arises from $H(t) = t \cdot \log(t) - t$. Emphasizing this distinction is important, also because we are now writing a "nonabelian sequel" to the present paper, namely on entropic regularization of semidefinite programming.

2 Varieties and Positivity

Let A be a $d \times n$ matrix of rank d with nonnegative integer entries and no zero column. We write L_A for the row space of A in \mathbb{R}^n . We associate two affine algebraic varieties with the matrix A. Both have strong positivity properties that makes them relevant for statistics and optimization. The reciprocal linear space R_A is the Zariski closure in \mathbb{C}^n of the set of points $v^{-1} = (v_1^{-1}, \ldots, v_n^{-1})$ where v ranges over vectors in L_A whose n coordinates are nonzero. The toric variety T_A is the Zariski cosure in \mathbb{C}^n of the set of points $\exp(v) = (\exp(v_1), \ldots, \exp(v_n))$ where v ranges over L_A . Both R_A and T_A are irreducible varieties of dimension d, defined over the field \mathbb{Q} of rational numbers. Their prime ideals live in the polynomial ring $\mathbb{Q}[x_1, \ldots, x_n]$.

The prime ideal of R_A has a distinguished universal Gröbner basis. It consists of the circuit polynomials. A circuit of A is a non-zero vector u of minimal support in kernel(A), assumed to have relatively prime integer coordinates. The corresponding circuit polynomial is the numerator of the rational function $\sum_{i=1}^{n} u_i/x_i$. This is due to Proudfoot and Speyer (cf. [9, Proposition 12]). The prime ideal of T_A is a toric ideal. It is generated by binomials

$$x^{u_+} - x^{u_-} = \prod_{i:u_i>0} x_i^{u_i} - \prod_{j:u_j<0} x_j^{-u_j},$$

where u runs over a finite set of integer vectors in kernel(A). This set is known in statistics as a $Markov\ basis$ for the matrix A. Here it usually does not suffice to consider only circuits.

We record the well-known formulas for the degrees of our two d-dimensional varieties. In what follows we use the notation $\operatorname{conv}(A) \subset \mathbb{R}^d$ for the convex hull of the columns of A viewed as points in \mathbb{R}^d , and $\operatorname{conv}(A \cup 0) \subset \mathbb{R}^d$ for the convex hull of $\operatorname{conv}(A)$ and the origin.

Proposition 3. The degree of the reciprocal linear space R_A is the Möbius number of the rank d matroid defined by the matrix A. This is bounded above by $\binom{n-1}{d-1}$, with equality when all $d \times d$ minors of A are non-zero. The degree of the toric variety T_A equals the normalized volume of the lattice polytope $\operatorname{conv}(A \cup 0)$. There is no upper bound in terms of d and n.

We refer to [9, Section 3] for the definition of the Möbius number. The fact that it gives the degree of R_A follows from the result of Proudfoot and Speyer stated above. The formula for the degree of an affine toric variety can be found in any textbook on toric geometry. For both varieties, consider the semialgebraic set of points with nonnegative real coordinates:

$$R_A^+ := R_A \cap \mathbb{R}^n_{\geq 0}$$
 and $T_A^+ := T_A \cap \mathbb{R}^n_{\geq 0}$. (6)

Our hypotheses on A ensure that these sets are Zariski dense in R_A and T_A respectively, so they have dimension d as well. We now identify A with the linear map $\mathbb{R}^n \to \mathbb{R}^d$, $v \mapsto Av$.

Proposition 4. Restricting the linear map A to the two sets in (6) defines homeomorphisms

$$R_A^+ \simeq \text{pos}(A)$$
 and $T_A^+ \simeq \text{pos}(A)$. (7)

The inverse map from the polyhedral cone on the right to the positive variety R_A^+ resp. T_A^+ on the left takes $b \in pos(A)$ to the analytic center resp. Birch point of the polytope $P_{A,b}$.

Proof. For each scenario, consider the map that takes $b \in pos(A)$ to the point $x^*(\infty)$ in $P_{A,b}$. This was defined in the Introduction as the solution to a convex optimization problem whose critical equations are polynomials. The map is well-defined and algebraic in both cases. The image equals T_A^+ resp. R_A^+ . Furthermore, we have $A \cdot x^*(\infty) = b$, so the composition with the linear map A is the identity on pos(A). This gives the desired homeomorphisms in (7). \square

We now fix a sufficiently generic vector $c \in \mathbb{Z}^n$ that serves as cost function in the linear program (1). We augment the matrix A by the row c to obtain a $(d+1) \times n$ matrix $\binom{A}{c}$. This has rank d+1, since c is generic. Let $R_{\binom{A}{c}}$ be the associated reciprocal variety, and let $T_{\binom{A}{c}}$ be the associated toric variety. Both of these live in \mathbb{C}^n , and they have dimension d+1. Propositions 3 and 4 hold for these varieties, with A replaced by $\binom{A}{c}$. We note that $R_{\binom{A}{c}}$ was called the *central sheet* in [9]. Its degree was computed in [9, Theorem 11]: it is the Möbius number $|\mu(A,c)|$. By contrast, Proposition 3 refers to the Möbius number $|\mu(A)|$.

The toric variety $T_{\binom{A}{c}}$ is the total space of the Gröbner degeneration of T_A given by c, as in [8, Section 9.4]. The degree of $T_{\binom{A}{c}}$ is the normalized volume of the convex hull of the n columns of $\binom{A}{c}$ together with the origin in \mathbb{R}^{d+1} . This volume is a subtle invariant which incorporates both geometric and arithmetic properties of the integer entries of A and c.

Example 5 (d=2,n=4). We consider the matrix $A=\begin{pmatrix} 3 & 2 & 1 & 0 \\ 0 & 1 & 2 & 3 \end{pmatrix}$. In our set-up, T_A is a toric surface in \mathbb{C}^4 , namely the cone over the *twisted cubic curve*. Its prime ideal is $\langle x_1x_3-x_2^2,x_1x_4-x_2x_3,x_2x_4-x_3^2\rangle$. The reciprocal surface R_A happens to be isomorphic to T_A . Its prime ideal is $\langle x_1x_2-3x_1x_4+2x_2x_4,2x_1x_3-3x_1x_4+x_3x_4,x_2x_3-2x_2x_4+x_3x_4\rangle$.

We now augment A by the cost vector $c = (c_1, c_2, c_3, c_4)$. The resulting varieties are hypersurfaces in \mathbb{C}^4 . The reciprocal variety $R_{\binom{A}{c}}$ is the affine cubic threefold defined by

$$\frac{x_1 x_2 x_3 x_4}{3} \cdot \det \begin{pmatrix} A \\ c \\ x^{-1} \end{pmatrix} = \begin{pmatrix} (c_1 - 3c_3 + 2c_4)x_1 x_3 x_4 + (c_1 - 2c_2 + c_3)x_1 x_2 x_3 \\ -(c_2 - 2c_3 + c_4)x_2 x_3 x_4 - (2c_1 - 3c_2 + c_4)x_1 x_2 x_4. \end{pmatrix}$$
(8)

The toric variety $T_{\binom{A}{c}}$ is an affine threefold in \mathbb{C}^4 , defined by an irreducible binomial such as

$$x_2^{c_1 - 3c_3 + 2c_4} x_4^{c_1 - 2c_2 + c_3} - x_1^{c_2 - 2c_3 + c_4} x_3^{2c_1 - 3c_2 + c_4}. (9)$$

The coefficients in (8) are the exponents in (9). The equation (9) is correct if and only if these exponents are relatively prime and nonnegative. In that case the degree of $T_{\binom{A}{c}}$ equals $2(c_1-c_2-c_3+c_4)$. Thus the degree depends on sign conditions and divisibilities in c. \diamond

We now define the curves of interest in linear programming by intersecting our varieties with the affine-linear spaces $\{x \in \mathbb{C}^n : Ax = b\}$, for $b \in \mathbb{R}^d$. The resulting curves are denoted

$$C_{A,b,c}^R = R_{\binom{A}{c}} \cap \{x : Ax = b\}$$
 and $C_{A,b,c}^T = T_{\binom{A}{c}} \cap \{x : Ax = b\}.$ (10)

Theorem 6. For generic vectors $b \in \mathbb{R}^d$ and $c \in \mathbb{Z}^n$, the intersections in (10) are curves in \mathbb{C}^n , namely the central curve and the entropic curve of the LP (1). Their degrees satisfy

$$\operatorname{degree}(\mathcal{C}_{A,b,c}^{R}) = |\mu(A,c)| \leq \binom{n-1}{d} \quad \text{and} \quad \operatorname{degree}(\mathcal{C}_{A,b,c}^{T}) \leq \operatorname{vol}(\operatorname{conv}(\binom{A}{c} \cup 0)). \tag{11}$$

Proof. The formula for the degree of the central curve $C_{A,b,c}^R$ appears in [9, Theorem 13]. The upper bound is attained when all maximal minors of the matrix $\binom{A}{c}$ are non-zero. The entropic curve $C_{A,b,c}^T$ is the intersection of the toric variety $T_{\binom{A}{c}}$ with $\{x:Ax=b\}$. The degree of $T_{\binom{A}{c}}$ equals $\operatorname{vol}(\operatorname{conv}(\binom{A}{c}\cup 0))$. Hence the inequality follows from Bézout's Theorem. This inequality can be strict, even when b and c are generic. See Proposition 10.

Remark 7. If n = d + 1 then Theorem 6 is trivial because $R_{\binom{A}{c}} = T_{\binom{A}{c}} = \mathbb{C}^n$. Note that $P_{A,b}$ is a line segment. The curves are straight lines, and all numbers in (11) are equal to 1. Indeed, the normalized volume of a simplex in the lattice generated by its vertices equals 1.

For applications in linear programming, we restrict our curves to the positive orthant:

$$C_{A,b,c}^{R,+} = R_{\binom{A}{c}}^+ \cap \{x : Ax = b\} \quad \text{and} \quad C_{A,b,c}^{T,+} = T_{\binom{A}{c}}^+ \cap \{x : Ax = b\}.$$
 (12)

These are real algebraic curves inside the polytope $P_{A,b}$. Following [9], we call $\mathcal{C}_{A,b,c}^{R,+}$ the central path of the linear program (1), and we call $\mathcal{C}_{A,b,c}^{T,+}$ the entropic path of (1). A slight distinction to [2, 9] is that our central path travels from the vertex of $P_{A,b}$ where c is minimized to the vertex where c is maximized, passing through the analytic center of $P_{A,b}$. For instance, Figure 1 in [9] shows all real points on the central curve. The central path is the piece inside the shaded hexagon $P_{A,b}$. That diagram illustrates the transportation problem in Example 1.

We now come to the parametrizations of our curves. These are understood by introducing scaled versions of the varieties R_A and T_A . We fix a cost vector $c \in \mathbb{R}^n$ which is generic in the sense that (1) has a unique optimal solution for all $b \in pos(A)$. Let ϵ be a positive real parameter, also assumed to be fixed for now. We consider the scaling $\frac{1}{\epsilon}c$ of the cost vector c.

Fix the affine-linear subspace $L_A - \frac{1}{\epsilon}c$ of \mathbb{R}^n . The reciprocal affine space $R_{A,c,\epsilon}$ is the Zariski closure in \mathbb{C}^n of the set of points $v^{-1} = (v_1^{-1}, \dots, v_n^{-1})$ where v ranges over vectors in $L_A - \frac{1}{\epsilon}c$ whose n coordinates are nonzero. The scaled toric variety $T_{A,c,\epsilon}$ is the Zariski cosure in \mathbb{C}^n of the set of points $\exp(v) = (\exp(v_1), \dots, \exp(v_n))$ where v ranges over $L_A - \frac{1}{\epsilon}c$.

Both $R_{A,c,\epsilon}$ and $T_{A,c,\epsilon}$ are irreducible affine varieties of dimension d. They are defined over appropriate subfields of the real numbers \mathbb{R} , namely the field $\mathbb{Q}(\epsilon)$ for $R_{A,c,\epsilon}$, and the field $\mathbb{Q}(z)$ for $T_{A,c,\epsilon}$, where $z = \exp(-1/\epsilon)$. If we abbreviate $z^c = (z^{c_1}, z^{c_2}, \dots, z^{c_n})$, then

$$T_{A,c,\epsilon} = z^c \star T_A. \tag{13}$$

Here \star denotes the Hadamard product, so $T_{A,c,\epsilon}$ is a torus translate of our toric variety T_A . We now present a generalization of Proposition 4, pertaining to the nonnegative varieties

$$R_{A,c,\epsilon}^+ := R_{A,c,\epsilon} \cap \mathbb{R}^n_{\geq 0} \quad \text{and} \quad T_{A,c,\epsilon}^+ := T_{A,c,\epsilon} \cap \mathbb{R}^n_{\geq 0}.$$
 (14)

These sets are Zariski dense in $R_{A,c,\epsilon}$ and $T_{A,c,\epsilon}$ respectively, so they have dimension d.

Theorem 8. Restricting the linear map A to the two sets in (14) defines homeomorphisms

$$R_{A,c,\epsilon}^+ \simeq \operatorname{pos}(A)$$
 and $T_{A,c,\epsilon}^+ \simeq \operatorname{pos}(A)$. (15)

The inverse map from the polyhedral cone on the right to the positive variety on the left takes $b \in pos(A)$ to the optimal point $x^*(\epsilon)$ of (2), where H(t) = log(t) resp. $H(t) = t \cdot log(t) - t$. For $\epsilon \to 0$, the homeomorphism approaches the regular triangulation of pos(A) given by c.

Proof. The strict convexity of the objective function in (2) ensures that the optimal solution $x^*(\epsilon)$ is the unique critical point of that function in $P_{A,b}$. The critical equations are those that define our varieties, and hence the singleton $\{x^*(\epsilon)\}$ is equal to $R_{A,c,\epsilon}^+ \cap P_{A,b}$ resp. $T_{A,c,\epsilon}^+ \cap P_{A,b}$. These two singletons are different, but they both converge to the same optimal vertex $x^*(0)$ of (1). The regular triangulation given by c is given combinatorially by the optimal bases as b ranges over pos(A). Each optimal basis specifies a d-dimensional face of the orthant $\mathbb{R}^n_{\geq 0}$, and the images of these cones triangulate pos(A). Both semialgebraic sets $R_{A,c,\epsilon}^+$ and $T_{A,c,\epsilon}^+$ converge, in the Hausdorff sense, to the fan that consists of these faces of $\mathbb{R}^n_{\geq 0}$. The linear map A induces a piecewise-linear isomorphism between that fan and the cone pos(A).

3 Optimal Transport

This section features a case study that is inspired by applications in machine learning [6, 12]. The classical Monge optimal transportation (OT) problem deals with the construction of optimal couplings for two given probability distributions. We explain how this problem, in its simplest version, can be written as a linear program (1). Many generalizations can be treated analogously; see e.g. [10, 11]. In Subsection 3.2 we carry this out for unbalanced OT.

3.1 The Classical Case

Given probability distributions $\mu \in \mathbb{R}^{d_1}_{\geq 0}$ and $\nu \in \mathbb{R}^{d_2}_{\geq 0}$ on the finite sets $[d_1] = \{1, \ldots, d_1\}$ and $[d_2] = \{1, \ldots, d_2\}$, and a cost matrix $c = (c_{\kappa, \lambda})_{\kappa \in [d_1], \lambda \in [d_2]} \in \mathbb{R}^{d_1 \times d_2}$, we aim to

minimize
$$\sum_{(\kappa,\lambda)\in[d_1]\times[d_2]} c_{\kappa,\lambda} \cdot x_{\kappa,\lambda}$$
 subject to $x \ge 0$ and (16)

$$\sum_{\lambda \in [d_2]} x_{\kappa,\lambda} = \mu_{\kappa} \text{ for all } \kappa \in [d_1] \text{ and } \sum_{\kappa \in [d_1]} x_{\kappa,\lambda} = \nu_{\lambda} \text{ for all } \lambda \in [d_2].$$
 (17)

We interpret μ_{κ} as the proportion of units of a product stored at $\kappa \in [d_1]$ and ν_{λ} as the proportion of units desired at $\lambda \in [d_2]$. Our goal is to transport all units from $[d_1]$ to $[d_2]$

with minimal transportation cost. The entry $c_{\kappa,\lambda}$ is the cost of transporting one unit from κ to λ . The feasible solutions $x = (x_{\kappa,\lambda})$ are known as transportation plans, or as couplings of μ and ν . Since $\|\mu\|_1 = \|\nu\|_1 = 1$, any solution x is a probability distribution on $[d_1] \times [d_2]$.

The matrix A for the linear program above has $d = d_1 + d_2 - 1$ rows and $n = d_1d_2$ columns, and its entries are in $\{0,1\}$. It represents the linear map that takes a $d_1 \times d_2$ matrix x to its vector $b = (\mu, \nu)$ of row sums and column sums. Here ν_{d_2} is deleted, so the rows of A are linearly independent. In OT theory it is customary to keep this redundancy. We saw the matrix A for $d_1 = 2$, $d_2 = 3$ in (5). The feasible region $P_{A,b}$ is a transportation polytope, consisting of all nonnegative $d_1 \times d_2$ matrices with fixed row and column sums. Every transportation polytope contains a unique rank one matrix x, namely the Birch point $x = (\mu_{\kappa} \cdot \nu_{\lambda})$ of $P_{A,b}$. This corresponds to an independent joint distribution.

The polytope underlying the cone pos(A) is the product $\Delta_{d_1-1} \times \Delta_{d_2-1}$ of two simplices. The triangulations of pos(A) are studied in [8, Section 6.2]. The toric variety T_A is the cone over the Segre variety $\mathbb{P}^{d_1-1} \times \mathbb{P}^{d_2-1}$. Its points are the $d_1 \times d_2$ matrices of rank at most 1. The prime ideal of T_A is generated by the 2×2 minors of a $d_1 \times d_2$ matrix; see [18, Example 5.1]. The positive variety T_A^+ represents the independence model for distributions on $[d_1]$ and $[d_2]$. We know from Proposition 4 that the linear map A identifies T_A^+ with the cone pos(A).

The same holds for the positive part R_A^+ of the reciprocal variety R_A . From a combinatorial perspective, it would be interesting to study this variety for OT in more detail. However, in the remainder of this paper we focus on the toric variety T_A instead. Here is the reason:

Remark 9. In machine learning one uses *entropic* regularization rather than *logarithmic* barrier regularization in (2). The former is more efficient than the latter. Thus, when d_1 and d_2 are large, the entropic path $\mathcal{C}_{A,b,c}^{T,+}$ is preferred to the central path $\mathcal{C}_{A,b,c}^{R,+}$. We refer to [6] for an explanation. Example 17 and the introduction of [20] offer details and references.

We next explain the degree drop which was observed for the entropic curve in Example 1.

Proposition 10. Let $b \in pos(A)$ and $c \in \mathbb{Z}^{d_1 \times d_2}$ where A is the matrix for OT. If $d_2 \geq 3$ then the upper bound in (11) for the degree of the entropic curve $C_{A,b,c}^T$ is always strict.

Proof. The trivial case $d_1 = d_2 = 2$ is covered by Remark 7. We have $d_2 \geq 3$, so $n = d_1 d_2$ is larger than $d+1 = d_1 + d_2$. Since T_A and $T_{\binom{A}{c}}$ are affine toric varieties in \mathbb{C}^n , we consider their closures \overline{T}_A and $\overline{T}_{\binom{A}{c}}$ in \mathbb{P}^n . We write $\{x_0 = 0\}$ for the hyperplane at infinity $\mathbb{P}^n \setminus \mathbb{C}^n$. We are

interested in the closure in \mathbb{P}^n of the entropic curve. This projective curve is denoted $\overline{\mathcal{C}}_{A,b,c}^T$. The upper bound on the right in (11) is the degree of the (d+1)-dimensional toric variety $\overline{T}_{\binom{A}{c}}$ in \mathbb{P}^n . We intersect $\overline{T}_{\binom{A}{c}}$ with the codimension d linear space $\{x \in \mathbb{P}^n : Ax = x_0b\}$. One of the irreducible components of this intersection is the curve $\overline{\mathcal{C}}_{A,b,c}^T$. By the general Bézout Theorem, the equation $\operatorname{degree}(\overline{\mathcal{C}}_{A,b,c}^T) = \operatorname{degree}(\overline{T}_{\binom{A}{c}})$ means that there is no component other than the entropic curve. Our goal is therefore to identify an extraneous component in

$$\overline{T}_{\binom{A}{c}} \cap \left\{ x \in \mathbb{P}^n : Ax = x_0 b \right\}. \tag{18}$$

Restricting to the hyperplane at infinity, we see that (18) contains

$$\overline{T}_A \cap \left\{ x \in \mathbb{P}^n : Ax = 0 \right\} \quad \supseteq \quad T_A \cap \left\{ x \in \mathbb{C}^n : Ax = 0 \right\}. \tag{19}$$

The affine variety on the right consists of all $d_1 \times d_2$ matrices of rank ≤ 1 whose rows and columns sum to zero. Such matrices have the form $x = (\mu_{\kappa} \cdot \nu_{\lambda})$ where $\mu \in \mathbb{C}^{d_1}$ and $\nu \in \mathbb{C}^{d_2}$ satisfy $\sum_{\kappa=1}^{d_1} \mu_{\kappa} = \sum_{\lambda=1}^{d_2} \nu_{\lambda} = 0$. This variety has dimension $d_1 + d_2 - 3 \geq 2$, so the intersection (18) has an extraneous component whose dimension exceeds that of $\mathcal{C}_{A,b,c}^T$. \square

Remark 11. Our proof reflects the special behavior we already know from the intersection

$$\overline{T}_A \cap \left\{ x \in \mathbb{P}^n : Ax = x_0 b \right\} \quad \supseteq \quad T_A \cap \left\{ x \in \mathbb{C}^n : Ax = b \right\}. \tag{20}$$

The toric variety T_A has degree $\binom{d_1+d_2-2}{d_1-1}$, but the intersection on the right has degree one. It is a single point, which is rational over $b=(\mu,\nu)$, namely the Birch point $x=(\mu_\kappa\cdot\nu_\lambda)$.

3.2 Unbalanced Case: Conic Coupling

Problem (16) is infeasible for optimal transport between measures μ and ν with $\|\mu\|_1 \neq \|\nu\|_1$. This unbalanced case is relevant in the statistical analysis of partial or incomplete data sets. One remedy is to replace the hard constraint (17) by a penalty function, e.g. Kullback-Leibler [4]. We here follow [5, 13] and present a linear programming formulation (1). In particular, this formulation can be understood as a moment constrained optimal transport problem.

Let us assume that, after discretization and scaling, the entries of the margins μ and ν are integers. This can be achieved up to arbitrary numerical precision. More precisely, we fix positive integers e_1 and e_2 such that $\mu_{\kappa} \in [e_1]$ for all $\kappa \in [d_1]$ and $\nu_{\lambda} \in [e_2]$ for all $\lambda \in [d_2]$.

We fix the state spaces $[d_1] \times [e_1]$ and $[d_2] \times [e_2]$. A joint probability distribution $x = (x_{\kappa,i,\lambda,j})$ on their product $([d_1] \times [e_1]) \times ([d_2] \times [e_2])$ is called a *conic coupling* for μ and ν if

$$\sum_{\lambda=1}^{d_2} \sum_{i=1}^{e_1} \sum_{j=1}^{e_2} i \, x_{\kappa,i,\lambda,j} = \mu_{\kappa} \text{ for } \kappa \in [d_1] \text{ and } \sum_{\kappa=1}^{d_1} \sum_{i=1}^{e_1} \sum_{j=1}^{e_2} j \, x_{\kappa,i,\lambda,j} = \nu_{\lambda} \text{ for } \lambda \in [d_2].$$
 (21)

We also assume that the cost function is extended to $c:([d_1]\times[e_1])\times([d_2]\times[e_2])\to\mathbb{R}$. The value $c_{\kappa,i,\lambda,j}$ is interpreted as the cost of generating j units of mass at $\lambda\in[d_2]$ from i units of mass at $\kappa\in[d_1]$. We propose the following relaxation of OT in the unbalanced case:

Minimize
$$\sum_{\substack{(\kappa,i,\lambda,j) \in \\ [d_1] \times [e_1] \times [d_2] \times [e_2]}} c_{\kappa,i,\lambda,j} \cdot x_{\kappa,i,\lambda,j} \text{ subject to } x \ge 0 \text{ and } (21).$$
 (22)

In the context of statistics, one can (but need not) impose the normalization constraint

$$\sum_{\substack{(\kappa,i,\lambda,j) \in \\ [d_1]\times[e_1]\times[d_2]\times[e_2]}} x_{\kappa,i,\lambda,j} = 1.$$
(23)

The minimizers x for the problem (22)-(23) are called *optimal conic couplings* of μ and ν . They define a cost-optimal random sampling mechanism of particle cluster pairs in $[d_1]$ and $[d_2]$ whose mean marginal empirical distributions are μ and ν , respectively. We next show that our formulation makes sense, meaning that conic couplings always exist.

Lemma 12. The linear program (22)-(23) is feasible for all $\mu \in [e_1]^{d_1}$ and all $\nu \in [e_2]^{d_2}$.

Proof. Let $\overline{\mu} = \frac{1}{\|\mu\|_1} \mu$ and $\overline{\nu} = \frac{1}{\|\nu\|_1} \nu$ be the induced probability distributions on $[d_1]$ and $[d_2]$. We define a probability distribution $x = (x_{\kappa,i,\lambda,j})$ on the space $[d_1] \times [e_1] \times [d_2] \times [e_2]$ by setting

$$x_{\kappa,i,\lambda,j} = \overline{\mu}_{\kappa} \cdot \delta_{\|\mu\|_{1},i} \cdot \overline{\nu}_{\lambda} \cdot \delta_{\|\nu\|_{1},j}. \tag{24}$$

Here we use Kronecker delta notation, i.e. $\delta_{a,b} = 1$ if a = b and $\delta_{a,b} = 0$ if $a \neq b$. The numbers in (24) are nonnegative. One checks that they satisfy both (21) and (23).

To connect to our general set up we write the linear program (22) in the standard form (1). In what follows we assume that $d_1, d_2, e_1, e_2 \geq 2$. The matrix A has $n = d_1e_1d_2e_2$ columns and $d = d_1 + d_2$ linearly independent rows. We identify \mathbb{C}^n with the space of tensors $x = (x_{\kappa,i,\lambda,j})$ of format $d_1 \times e_1 \times d_2 \times e_2$. The column of A indexed by (κ, i, λ, j) is the vector $i\mathbf{e}_{\kappa} \oplus j\mathbf{e}_{\lambda}$ in $\mathbb{N}^d = \mathbb{N}^{d_1} \oplus \mathbb{N}^{d_2}$, where \mathbf{e}_{κ} and \mathbf{e}_{λ} denote unit vectors. If we set $b = (\mu, \nu)^T \in \mathbb{R}^d$ then the polytope $P_{A,b}$ consists of all nonnegative tensors x that satisfy the linear constraints (21).

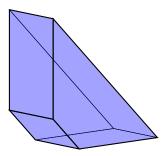


Figure 1: The 4-dimensional cone pos(A) in Example 13 has a slanted cube for its base.

Example 13 $(d_1 = e_1 = d_2 = e_2 = 2)$. Our matrix has d = 4 rows and n = 16 columns:

We identify \mathbb{C}^{16} with the space of $2 \times 2 \times 2 \times 2$ -tensors $x = (x_{\kappa,i,\lambda,j})$. The coordinates $x_{1111}, x_{1112}, \dots, x_{2222}$ are ordered lexicographically, which matches the column ordering of A. The toric variety X_A has dimension 4 and degree 72 in \mathbb{C}^{16} . The prime ideal of X_A is homogeneous with respect to the column sum grading (2, 3, 2, 3, 3, 4, 3, 4, 2, 3, 2, 3, 3, 4, 3, 4). It is minimally generated by 39 binomials: 5 of degree 4, 8 of degree 5, 18 of degree 6, and 8 of degree 7. The polyhedral cone pos(A) is spanned by 8 rays, and it has 6 facets. Explicitly,

$$pos(A) = \left\{ b \in \mathbb{R}^4_{>0} : b_1 + b_2 \le 2b_3 + 2b_4 \text{ and } b_3 + b_4 \le 2b_1 + 2b_2 \right\}.$$
 (26)

This is the cone over a polytope combinatorially isomorphic to a 3-cube, shown in Figure 1. The vertices of that cube correspond to the eight columns of A with entries 0, 0, 1, 2.

4 Polytopes and their Volumes

The entropic method for solving the linear program (1) is a two-step process. First, the solution $x^*(\epsilon)$ to the regularized problem (2) is computed. Here, $\epsilon > 0$ and $H(t) = t \log(t) - t$. Second, one lets $\epsilon \to 0$ and tracks the minimizer $x^*(\epsilon)$ to the optimal vertex $x^*(0)$ of $P_{A,b}$.

Step 1 amounts to solving the polynomial system given by Ax = b and $x \in T_{A,c,\epsilon}$. For linear programming, one wants the unique positive solution $x^*(\epsilon)$. But, for other applications, e.g. scattering amplitudes in particle physics [19], all complex solutions are needed. A standard method for finding them all is homotopy continuation [17]. We expect the number of solutions to be deg $T_{A,c,\epsilon} = \text{vol}(\text{conv}(A \cup 0))$, and this is the number of paths to be tracked. This number is also the algebraic degree of $x^*(\epsilon)$, over the ground field $\mathbb{Q}(z)$ in (13).

Numerical algebraic geometry interfaces gracefully with interior point methods in optimization. In a scenario where the matrix A is fixed and (2) must be solved for many different vectors b and c, it makes sense to initialize by computing all complex solutions. This needs to be done *only once*. Indeed, for new parameters b', c', one can use $x^*(\epsilon) \in T_{A,c,\epsilon} \cap \{Ax = b\}$ as a start solution to find the positive point in $T_{A,c',\epsilon} \cap \{Ax = b'\}$. We will come back to continuation methods at the end of Section 5, in our discussion of step 2, in which $\epsilon \to 0$.

Given an interesting matrix A, the reasons above motivate the combinatorial problem of finding the degree of $T_{A,c,\epsilon}$. This means finding the volume of the polytope $\operatorname{conv}(A \cup 0)$. We here solve this problem for unbalanced optimal transport, as formulated in Subsection 3.2.

Let A be the $d \times n$ matrix for conic coupling (22), where $d = d_1 + d_2$ and $n = d_1e_1d_2e_2$. For any right hand side $b = (b_1, \ldots, b_{d_1}, b_{d_1+1}, \ldots, b_{d_2})^T$, the set of feasible solutions is the polytope $P_{A,b}$. We know that $P_{A,b} \neq \emptyset$ if and only if $b \in pos(A)$, and $dim(P_{A,b}) = n - d$ if and only if b is in the interior of pos(A). Our next result characterizes that cone, as in (26).

Proposition 14. The feasibility cone pos(A) for the conic coupling problem (22) equals

$$\{y \in \mathbb{R}^d_{>0} : y_1 + \dots + y_{d_1} \le e_1(y_{d_1+1} + \dots + y_{d_1+d_2}), y_{d_1+1} + \dots + y_{d_1+d_2} \le e_2(y_1 + \dots + y_{d_1})\}.$$

This d-dimensional cone has $2d_1d_2$ rays and $d_1 + d_2 + 2$ facets. It is the cone over a simple (d-1)-dimensional polytope which is combinatorially isomorphic to the product of simplices

$$\Delta_1 \times \Delta_{d_1-1} \times \Delta_{d_2-1}$$
.

Proof. Let K be the polyhedral cone given in the assertion. Every column vector $i\mathbf{e}_{\kappa} \oplus j\mathbf{e}_{\lambda}$ of the matrix A lies in K because $0 \le i \le je_1$ and $0 \le j \le ie_2$. Hence $pos(A) \subseteq K$. For the reverse inclusion, we identify the extreme rays of K. Every vector in K must have at least one positive coordinate among the first d_1 coordinates and ditto for the last d_2 coordinates. We see that at most d-2 of the nonnegativity constraints can be attained. Thus every extreme ray must attain equality in at least one of the other inequalities. This implies that the extreme rays are $\mathbf{e}_{\kappa} \oplus e_2 \mathbf{e}_{\lambda}$ for some $\kappa \in [d_1]$ and $e_1 \mathbf{e}_{\kappa} \oplus \mathbf{e}_{\lambda}$ for some $\lambda \in [d_2]$.

The following result pertains to the affine variety T_A . Its proof is analogous to that above.

Proposition 15. The d-dimensional polytope $conv(A \cup 0)$ has d+4 facets, given by the d+2 inequalities defining pos(A), together with $y_1 + \cdots + y_{d_1} \leq e_1$ and $y_{d_1+1} + \cdots + y_{d_1+d_2} \leq e_2$.

Solving the entropic regularization (2) for (22) means intersecting the polytope $P_{A,b}$ with the scaled toric variety $T_{A,c,\epsilon} = z^c \star T_A$, where $z = \exp(-1/\epsilon)$. Algebraically, we compute the unique positive solution $x = x^*(\epsilon)$ to the following equations, with $H(t) = t \cdot \log(t) - t$:

$$Ax = b$$
 and $\operatorname{rank}\begin{pmatrix} A \\ c + \epsilon H'(x) \end{pmatrix} \le d + 1.$ (27)

The algebraic degree of (27) is the number of solutions in \mathbb{C}^n . This is the degree over \mathbb{Q} of the floating point numbers that are output by any numerical algorithm. It is bounded above by

$$\operatorname{degree}(T_{A,c,\epsilon}) = \operatorname{degree}(T_A) = \operatorname{vol}(\operatorname{conv}(A \cup 0)). \tag{28}$$

Our main result is a formula in terms of d_1, e_1, d_2, e_2 for this algebraic complexity measure. In other words, we generalize the number 72, which is the degree of $T_A \subset \mathbb{C}^{16}$ in Example 13.

Theorem 16. The algebraic degree of the constraints (27) for optimal conic coupling is

$$\operatorname{degree}(T_A) = \binom{d_1 + d_2}{d_1} \left((e_1^{d_1} - 1)(e_2^{d_2} - 1) + \frac{d_1}{d_1 + d_2}(e_2^{d_2} - 1) + \frac{d_2}{d_1 + d_2}(e_1^{d_1} - 1) \right). \tag{29}$$

To illustrate our formula, consider the binary case $(d_1 = d_2 = 2)$, where it gives $\binom{4}{2}(9 + \frac{2}{4}3 + \frac{2}{4}3) = 72$, and the ternary case $(d_1 = d_2 = 3)$, where $\binom{6}{3}(26^2 + \frac{3}{6}26 + \frac{3}{6}26) = 14040$.

Proof. We compute the volume in (28). Fix integers $d, e \geq 2$ and consider the d-polytope

$$P_{d,e} = \text{conv}\{k\mathbf{e}_i : i = 1, \dots, d \text{ and } k = 1, \dots, e\}.$$

The normalized volume of this polytope is e^d-1 . The convex hull of the columns of A equals

$$\operatorname{conv}(A) = P_{d_1,e_1} \times P_{d_2,e_2}.$$

The normalized volume of a direct product is multiplicative up to a binomial coefficient, so

$$\operatorname{vol}(\operatorname{conv}(A)) = \binom{d_1 + d_2}{d_1} \operatorname{vol}(P_{d_1, e_1}) \operatorname{vol}(P_{d_2, e_2}) = \binom{d_1 + d_2}{d_1} (e_1^{d_1} - 1) (e_2^{d_2} - 1). \tag{30}$$

This explains the first summand in (29). It remains to determine the volume of the region $conv(A \cup 0) \setminus conv(A)$. To this end, we consider the facets of conv(A) that are visible from the origin 0. There are precisely two such facets, and they are defined respectively by

$$y_1 + \dots + y_{d_1} = 1$$
 and $y_{d_1+1} + \dots + y_{d_2} = 1$. (31)

These two facets are the (d_1+d_2-1) -dimensional polytopes $\Delta_{d_1-1} \times P_{d_2,e_2}$ and $P_{d_1,e_1} \times \Delta_{d_2-1}$. Since the origin has lattice distance one from the hyperplanes (31), the volume of the region $\operatorname{conv}(A \cup 0) \setminus \operatorname{conv}(A)$ coincides with the sum of the volumes of the two polytopes:

$$\operatorname{vol}(\Delta_{d_1-1} \times P_{d_2,e_2}) + \operatorname{vol}(P_{d_1,e_1} \times \Delta_{d_2-1}) = {\binom{d_1+d_2-1}{d_2}}(d_2^{e_2}-1) + {\binom{d_1+d_2-1}{d_1}}(d_1^{e_1}-1).$$

This gives the last two summands in (29), and the proof is complete.

5 Computational Schemes

We now turn to convex optimization methods for solving (2). Recall that $H(t) = t \cdot \log(t) - t$ and hence $H^*(s) = \exp(s)$ in the dual formulation. We can solve (3) using coordinate ascent, i.e. by iteratively optimizing each variable p_i in (3) in a cyclic order. In statistics, this is known as *iterative proportional scaling* (IPS, see [7, 16]). This method converges linearly [14]. Randomized iterations over the p_i can further improve the performance. When each one-dimensional optimization is computationally cheap, this method is particularly interesting.

Example 17 (Sinkhorn iterations). For classical optimal transport (16), coordinate ascent is the well-known $Sinkhorn \ algorithm \ [3, 6, 12]$. It uses highly efficient matrix-vector products. Writing $(f_{\kappa})_{\kappa \in [d_1]}$ and $(g_{\lambda})_{\lambda \in [d_2]}$ for the dual variables, the dual OT problem (3) reads:

Maximize
$$\sum_{\kappa=1}^{d_1} \mu_{\kappa} f_{\kappa} + \sum_{\lambda=1}^{d_2} \nu_{\lambda} g_{\lambda} - \epsilon \cdot \sum_{\kappa=1}^{d_1} \sum_{\lambda=1}^{d_2} \exp((f_{\kappa} + g_{\lambda} - c_{\kappa,\lambda})/\epsilon).$$
 (32)

It is easy to solve this for each variable separately. Equating derivatives to zero, we find

$$f_{\kappa} = -\epsilon \cdot \log \left(\sum_{\lambda=1}^{d_2} \exp((g_{\lambda} - c_{\kappa,\lambda})/\epsilon) \right) + \epsilon \cdot \log(\mu_{\kappa}) \text{ and similarly for } g_{\lambda}.$$
 (33)

Sinkhorn iteration means executing these assignments. A useful reformulation is obtained by setting $F_{\kappa} = \exp(f_{\kappa}/\epsilon)$, $G_{\lambda} = \exp(f_{\lambda}/\epsilon)$, and $K_{\kappa,\lambda} = \exp(-c_{\kappa,\lambda}/\epsilon)$. Here F is a row vector, and G is a column vector. With this, the rules for updating F and G are $F_{\kappa} = \mu_{\kappa}/[K \cdot G]_{\kappa}$ and $G_{\lambda} = \nu_{\lambda}/[F \cdot K]_{\lambda}$. The primal solution is the matrix $x = \operatorname{diag}(F) \cdot K \cdot \operatorname{diag}(G)$. These steps are highly parallelizable, so large-scale problems can be solved effectively. This explains the preference for entropic regularization in Remark 9.

Coordinate ascent can be applied for any matrix A, but in general there is no simple formula for the one-variable updates. But, we can resort to non-linear optimization for this.

Example 18 (Coordinate ascent for entropic conic transport). The dual problem for (22) is

Maximize
$$h + \sum_{\kappa=1}^{d_1} \mu_{\kappa} f_{\kappa} + \sum_{\lambda=1}^{d_2} \nu_{\lambda} g_{\lambda} - \epsilon \cdot \sum_{\kappa, \lambda, i, j} \exp((h + i f_{\kappa} + j g_{\lambda} - c_{\kappa, i, \lambda, j})/\epsilon).$$
 (34)

Here we also assumed (23), and h is the dual variable for that normalization constraint. Coordinate ascent means that we compute, for each κ , the unique positive solution F_{κ} to

$$\sum_{i=1}^{d_1} i \cdot \gamma_{\kappa,i} \cdot (F_\kappa)^i = \mu_\kappa \,, \tag{35}$$

where $\gamma_{\kappa,i} = \sum_{\lambda,j} \exp((h+jg_{\lambda}-c_{\kappa,i,\lambda,j})/\epsilon)$. This step is more costly than applying (33). \diamond

Solving (35) is costly. One prefers cheap iterations, inspired by first-order methods. Of special interest is the Darroch-Ratcliff algorithm [7], which is also known as *generalized iterative scaling* (GIS). This was recognized in [16] as an instance of majorization-minimization on the dual formulation (3). GIS is a remarkably simple iterative process. As with Sinkhorn, each step involves d matrix-vector products. See [3, Figure 4] for the connection. Theorem 19 below shows that GIS can be used¹ effectively for conic coupling (22)-(23).

Before starting the iteration, we modify A, b and c slightly. To match [7], we formulate an equivalent linear program where all columns of A have the same sum. For this conversion, we require that the all-ones vector $(1, \ldots, 1)$ is in the row space L_A . In geometric terms, this means that T_A is the affine cone over a projective toric variety. The matrix A for classical OT satisfies this assumption. In the unbalanced case, it holds after we add the constraint (23).

We now assume $(1, ..., 1) \in L_A$. Fix $b \in pos(A)$. Then $s = \sum_{i=1}^n x_i$ is fixed for $x \in P_{A,b}$. Let a be the maximum among the column sums of A. To each column a_j , we append the entry $a_{d+1,j} = a - |a_j|$, where $|a_j| = \sum_{i=1}^d a_{ij}$. Prepending the column (0, ..., 0, a), we obtain

$$\mathcal{A} = \begin{bmatrix} 0 & A \\ a & a_{d+1,1} & \cdots & a_{d+1,n} \end{bmatrix} \in \mathbb{N}^{(d+1)\times(n+1)}.$$

Note that the entries in each column of \mathcal{A} sum to a. Let $s_c = 1 + \sum_{i=1}^n \exp(-c_i/\epsilon)$, and

$$\beta = \left(\frac{b}{s+1}, \ a - \frac{|b|}{s+1}\right)^{\top}$$
 and $\gamma = \left(\epsilon \log(s_c), \ c_1 + \epsilon \log(s_c), \dots, \ c_n + \epsilon \log(s_c)\right)$.

These data define the following variant of the regularized linear program (2):

Minimize
$$\gamma \cdot y + \epsilon \sum_{i=0}^{n} H(y_i)$$
 subject to $\mathcal{A} y = \beta$ and $y \ge 0$. (36)

We now rephrase the result of Darroch and Ratcliff [7] in the geometric setting of Section 2. An essentially equivalent formulation was presented recently in [3, Proposition 5.1].

Theorem 19. If (2) is feasible, then the solution $x^*(\epsilon)$ is given by $(y_1/y_0, \ldots, y_n/y_0)$, where $y = y^*(\epsilon) \in \mathbb{R}^{n+1}_{\geq 0}$ is the unique solution to (36). That is, y is the unique point in $T^+_{\mathcal{A},\gamma,\epsilon} \cap \{\mathcal{A}y = \beta\}$. It satisfies $\sum_{i=0}^n y_i = 1$ and is obtained as the unique limit point of the iteration

$$y^{(0)} = z^{\gamma} := \exp(-\gamma/\epsilon), \qquad y_i^{(k+1)} = y_i^{(k)} \left(\frac{\beta^{a_i}}{(\mathcal{A}y^{(k)})^{a_i}}\right)^{\frac{1}{a}} \quad \text{for } k \to \infty.$$
 (37)

Proof. Since $\sum_{i=0}^{n} \beta_i = a$, every solution y to (36) satisfies $\sum_{i=0}^{n} y_i = 1$. Consider the map $\iota: (x_1, \ldots, x_n) \mapsto \frac{1}{|x|+1} (1, x_1, \ldots, x_n)$. The map sending b to β is such that the diagram

$$T_{A,c,\epsilon}^{+} \stackrel{\iota}{\longleftarrow} T_{A,\gamma,\epsilon}^{+} \cap \Delta_{n}$$

$$\downarrow \qquad \qquad \downarrow$$

$$pos(A) \xrightarrow{b \mapsto \beta} conv(A)$$

¹An illustration of entropic conic unbalanced OT, for numerical comparison between GIS, IPS and general purpose convex optimization, is implemented at https://github.com/fxv27/EntropicConicUOT

is commutative. Here the vertical maps correspond to the isomorphism $T_{A,c,\epsilon}^+ \simeq \text{pos}(A)$ in Theorem 8. The diagram shows that (36) has the solution $y = y^*(\epsilon) = \iota(x^*(\epsilon))$. The iteration (37) and its convergence can be derived from the proof of [7, Theorem 1].

The geometric interpretation of Theorem 19 is shown in Figure 2. The linear map given by \mathcal{A} sends the probability simplex Δ_n onto the polytope $\operatorname{conv}(\mathcal{A})$. Note that z^{γ} lies in Δ_n . The polytope $P_{\mathcal{A},\beta}$ is the set of all points in Δ_n that map to $\beta \in \operatorname{conv}(\mathcal{A})$ under \mathcal{A} . It is shown as a green triangle. The toric variety $T_{\mathcal{A},\gamma,\epsilon}$ inside Δ_n is shown in blue, and $\operatorname{conv}(\mathcal{A})$ is the red line segment. The point $z^{\gamma} = y^{(0)}$ lies on $T_{\mathcal{A},\gamma,\epsilon}$ and is updated throughout the iteration. The solution $y = y^*(\epsilon) = \lim_{k \to \infty} y^{(k)}$ to (36) is the unique point in $T_{\mathcal{A},\gamma,\epsilon} \cap P_{\mathcal{A},\beta}$.

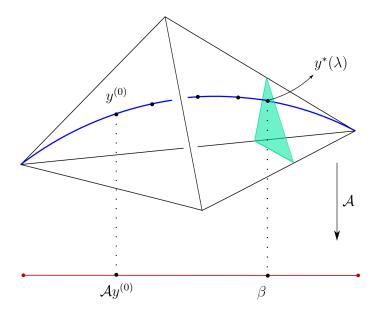


Figure 2: Illustration of the GIS algorithm from Theorem 19.

We now turn to the second step of the entropic interior point method, which consists of tracking $x^*(\epsilon)$ to the optimal vertex $x^*(0)$ of $P_{A,b}$. We assume that c is sufficiently generic, so that $x^*(0)$ is indeed a vertex. Observe that, for all $\mu \in (0, \epsilon]$, we have $x^*(\mu) > 0$, $A x^*(\mu) = b$ and $x^*(\mu) \in T_{A,c,\mu}$. Equivalently, $x^*(\mu) = (t(\mu)^{a_j})_{j=1,\dots,n}$, where $t(\mu) \in \mathbb{R}^d_{>0}$ is such that

$$\sum_{j=1}^{n} a_{ij} \exp(-c_j/\mu) t(\mu)^{a_j} = b_i \quad \text{for } i = 1, \dots, d.$$
(38)

The resulting functions $t(\mu)^{a_j}$ parametrize the entropic path for $\mu \in (0, \epsilon]$. The starting point $t(\epsilon)$ is found by solving the binomial equations $x^*(\epsilon)_j = t(\epsilon)^{a_j}$, $j = 1, \ldots n$. This can be done by a Smith normal form computation. The tracking for $\mu \to 0^+$ is carried out with standard predictor-corrector techniques from numerical homotopy continuation [17, Section 2.3].

We conclude with a toric interpretation of the homotopy (38). For $\mu = \epsilon > 0$, each of the Laurent polynomials in (38) defines a hypersurface in the projective toric variety Y_P associated to the polytope $P = \text{conv}(A \cup 0)$. There are vol(P) many solutions to (38) in

 Y_P , one of which gives $x^*(\epsilon)$. For $\mu \to 0$, this positive solution drifts to a lower dimensional torus orbit in Y_P , indicating which inequalities in $x^*(0) \ge 0$ are active. Identifying this orbit can be done by tracking the homotopy path $t(\mu)$ in homogeneous coordinates on Y_P .

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