Lecture 3: Maximum Entropy Convex Programs and TSP

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Disclaimer: *These notes have not been subjected to the usual scrutiny reserved for formal publications.*

Given a polynomial

$$p(z_1, \dots, z_n) = \sum_{\kappa \in \mathbb{Z}_{\geq 0}} c_p(\kappa) z^\kappa,$$

where $c_p(\kappa)$ is the coefficient of z^κ in p, the *Newton polytope* of p is the convex hull of all integer vectors κ with non-zero coefficient,

$$\text{Newt}(p) := \text{conv}\{\kappa \in \mathbb{Z}_{\geq 0} : c_p(\kappa) \neq 0\}$$

For example, if p is the generating polynomial of all spanning trees of a graph G, $\sum_T z^T$, then Newt(p) is the spanning tree polytope of G, the convex hull of the indicator vectors of all spanning trees of G.

In this section, we study a generalization of Gurvits' convex program:

$$\inf_{z>0} \frac{p(z_1, \dots, z_n)}{z^\alpha} \tag{3.1}$$

where $\alpha \in \mathbb{R}^n_{\geq 0}$.

Lemma 3.1. *For any polynomial $p \in \mathbb{R}_{\geq 0}[z_1, \dots, z_n]$, and any $\alpha \in \mathbb{R}^n_{\geq 0}$, we have $\inf_{z>0} \frac{p(z)}{z^\alpha} > 0$ iff $\alpha \in$ Newt(p).*

Proof. $\Leftarrow$: First, assume that $\alpha \in$ Newt(p). Then, there is a convex combination of the vertices of this polytope that is equal to α,

$$\alpha = \sum_{\kappa : c_p(\kappa) \neq 0} \lambda_\kappa \kappa$$

where $\sum_\kappa \lambda_\kappa = 1$ and each $\lambda_\kappa \geq 0$. Then, for any $z > 0$ we can write,

$$p(z) = \sum_{\kappa \in \mathbb{Z}^n_{\geq 0}} \lambda_\kappa \frac{c_p(\kappa) z^\kappa}{\lambda_\kappa} \geq \prod_{\kappa \in \mathbb{Z}^n_{\geq 0}} \left(\frac{c_p(\kappa) z^\kappa}{\lambda_\kappa} \right)^{\lambda_\kappa} = z^\alpha \prod_{\kappa \in \mathbb{Z}^n_{\geq 0}} \left(\frac{c_p(\kappa)}{\lambda_\kappa} \right)^{\lambda_\kappa},$$

where the inequality follows by the weighted AM-GM inequality and that $c_p(\kappa) \geq 0$ and $z > 0$. Therefore, $\inf_{z>0} \frac{p(z)}{z^\alpha} \geq \prod_{\kappa \in \mathbb{Z}^n} \left(\frac{c_p(\kappa)}{\lambda_\kappa} \right)^{\lambda_\kappa} > 0$ as desired.

$\Rightarrow$: Conversely, suppose $\alpha \notin$ Newt(p). Then, there exists a separating hyperplane, i.e., there exists $c \in \mathbb{R}^n$ such that $\langle c, \alpha \rangle > b$ and $\langle c, x \rangle \leq b$ for any $x \in$ Newt(p) for some $b \in \mathbb{R}$. Suppose $\langle c, \alpha \rangle \geq b + \epsilon$ for some $\epsilon > 0$. Now, let $z^* = \exp(tc)$ where $t > 0$ is a sufficiently large number. Then,

$$\begin{aligned}
\inf_{z>0} \frac{p(z)}{z^\alpha} &\leq \frac{p(z^*)}{{z^*}^\alpha} \\
&= \frac{\sum_{\kappa \in \mathbb{Z}^n_{\geq 0}} c_p(\kappa) e^{\langle \log z^*, \kappa \rangle}}{e^{\langle \log z^*, \alpha \rangle}} \\
&= \frac{\sum_{\kappa \in \mathbb{Z}^n_{\geq 0}} c_p(\kappa) \exp(t \langle c, \kappa \rangle)}{\exp(t \langle c, \alpha \rangle)} \leq \frac{\sum_{\kappa \in \mathbb{Z}^n_{\geq 0}} c_p(\kappa) \exp(tb)}{\exp(t(b + \epsilon)}
\end{aligned}$$

Letting $t \to \infty$ the RHS converges to 0. □

Some remarks are in order: Recall that in lecture 2 we proved Gurvits' theorem that for any real stable $p \in \mathbb{R}_{\geq 0}[z_1, \ldots, z_n]$,

$$\partial_{z_1} \ldots \partial_{z_n} p|_{z=0} \geq e^{-n} \inf_{z>0} \frac{p(z)}{z_1 \ldots z_n}$$

The RHS is a special case of (3.1) when $\alpha = \mathbf{1}$. If the RHS is positive, then by the above lemma, $\mathbf{1} \in \text{Newt}(p)$. In such a case Gurvits' theorem implies that the coefficient of $z^{\mathbf{1}}$ is non-zero in p. More generally, this is true for any integer point in Newton polytopes of real stable polynomials: Given any real stable polynomial $p \in \mathbb{R}_{\geq 0}[z_1, \ldots, z_n]$, and any $\alpha \in \mathbb{Z}^n$ such that $\alpha \in \text{Newt}(p)$, we have $c_p(\alpha) > 0$.

Next, we prove the following theorem:

Theorem 3.2. *Let $\mu : 2^{[n]} \to \mathbb{R}_{\geq 0}$ be a probability distribution. Let $\alpha \in Newt(g_\mu)$. Then, there exists an external field $(\lambda_1, \ldots, \lambda_n)$ such that for any $1 \leq i \leq n$,*

$$\mathbb{P}_{\lambda * \mu}[i] = \alpha_i,$$

i.e., the marginal probability of i under the distribution $\mu * \lambda$ is α_i.

The above theorem conceptually has a very important message. Say μ is a strongly Rayleigh distribution. It says that given any point α in the Newton polytope of g_μ, there is *another strongly Rayleigh distribution* μ' such that the marginals of μ' is equal to α.

Remark 3.3. *We remark that if α is in the interior of the Newton polytope we can attain α exactly, otherwise, we can only satisfy α as a marginal approximately, i.e., we can find a sequence of external field vectors $\lambda^1, \lambda^2, \ldots$ such that the marginal vectors of the distributions $\mu * \lambda^1, \mu * \lambda^2, \ldots$ converge to α.*

Recall that many of the probabilistic operations on μ can be translated to operations on the generating polynomial g_μ. To prove the theorem, it is natural to write down the marginal vector of a distribution μ: For any $1 \leq i \leq n$ we can write

$$\mathbb{P}_{S \sim \mu}[i \in S] = \partial_{z_i} g_\mu(z)\,|_{z=1}\,.$$

Sometimes, it is cleaner to assume g_μ is not normalized to $g_\mu(\mathbf{1}) = 1$. In such a case, we can write

$$\mathbb{P}_{S \sim \mu}[i \in S] = \left.\frac{\partial_{z_i} g_\mu(z)}{g_\mu(z)}\right|_{z=\mathbf{1}} = \partial_{z_i} \log g_\mu(z)\,|_{z=\mathbf{1}}\,. \tag{3.2}$$

We write the following convex reformulation of the program given in (3.1) and we study its optimality condition.

$$\inf_y \log \frac{g_\mu(e^{y_1}, \ldots, e^{y_n})}{e^{\langle y, \alpha \rangle}}. \tag{Max-Entropy CP}$$

In particular, the above program can be obtained by a change of variables $z_i \leftrightarrow e^{y_i}$ and taking log of the objective value.

Since the above convex program has no constraints, the optimum solution is attained unless the optimum value is $-\infty$. In Lemma 3.1 we argued that the above infimum is $-\infty$ iff $\alpha \notin \text{Newt}(p)$. So, since $\alpha \in \text{Newt}(p)$, the infimum is bounded and we assume y^* is (an) optimum solution.

Since y^* is an optimal solution, the Gradient of the convex function must be zero at y^*; so for each $1 \leq i \leq n$ we can write

$$0 = \partial_{y_i} \left(\log g_\mu(e^{y_1}, \ldots, e^{y_n}) - \langle y, \alpha \rangle \right)|_{y=y^*}$$

Therefore,

$$\frac{\partial_{y_i} g_\mu(e^{y_1}, \ldots, e^{y_n})}{g_\mu(e^{y_1}, \ldots, e^{y_n})}\Big|_{y=y^*} = \alpha_i \tag{3.3}$$

Letting $\lambda = e^{y^*}$, i.e., $\lambda_i = e^{y_i^*}$ for all i, observe that

$$\begin{aligned} g_\mu(e^{y_1}, \ldots, e^{y_n})|_{y=y^*} &= g_\mu(\lambda_1 z_1, \ldots, \lambda_n z_n)_{z=\mathbf{1}}, \\ \partial_{y_i} g_\mu(e^{y_1}, \ldots, e^{y_n})|_{y=y^*} &= \partial_{z_i} g_\mu(\lambda_1 z_1, \ldots, \lambda_n z_n)|_{z=\mathbf{1}}. \end{aligned}$$

Therefore, by (3.2) for any $1 \le i \le n$,

$$\mathbb{P}_{S\sim\lambda*\mu}[i] = \partial_{z_i} \log g_{\lambda*\mu}(z)|_{z=\mathbf{1}} = \frac{\partial_{z_i} g_\mu(\lambda_1 z_1, \ldots, \lambda_n z_n)}{g(\lambda_1, \ldots, \lambda_n)}\Big|_{z=\mathbf{1}} = \alpha_i,$$

as desired. The last identity follows by (3.3)

(Max-Entropy CP) is called the maximum entropy convex program. This can be seen as a generalization of the convex program proposed by Gurvits that we discussed in Lecture 3. To computationally solve (Max-Entropy CP) we need to be able to evaluate the generating polynomial of μ and evaluate its partial derivatives. If μ is a strongly Rayleigh distribution, we can approximately evaluate g_μ. To be precise, one also needs to study the bit precision of the optimum solution y^*. It is a-priori unclear if the optimal solution y^* can be represented (or approximated) by polynomially (in n) many bits. This questions is well studied [Asa+17; SV14; SV19] and it is not in the scope of this course.

3.1 Dual of Max-Entropy CP

Let $p \in \mathbb{R}_{\ge 0}[z_1, \ldots, z_n]$ and let $\alpha = \text{Newt}(p)$. Consider the following convex program:

$$\begin{aligned} \max \quad & \sum_{\kappa\in\text{Newt}(p)} q_\kappa \log \frac{c_p(\kappa)}{q_\kappa} \\ \text{s.t.,} \quad & \sum_{\kappa\in\text{Newt}(p)} q_\kappa \kappa_i = \alpha_i \qquad \forall 1 \le i \le n, \\ & \sum_\kappa q_\kappa = 1 \\ & q_\kappa \ge 0 \qquad\qquad \forall \kappa. \end{aligned} \tag{Max-Entropy Dual}$$

We claim this is the dual to (Max-Entropy CP). We think of q as a distribution over integer points in Newt(p). To write the dual of this program, we first need to write the Lagrangian:

$$\max_{q>0} \inf_{y\in\mathbb{R}^n} L(q,\gamma) = \max_{q>0} \inf_{y} \sum_{\kappa\in\text{Newt}(p)} q_\kappa \log\frac{c_p(\kappa)}{q_\kappa} - \sum_{i=1}^n y_i \left(\alpha_i - \sum_{\kappa\in\text{Newt}(p)} q_\kappa\kappa_i\right) - s\left(1 - \sum_{\kappa\in\text{Newt}(p)} q_\kappa\right)$$

By strong duality we can substitute the max and inf, so

$$\max_{q>0} \inf_{y\in\mathbb{R}^n, s} L(q,\gamma,s) = \inf_{y\in\mathbb{R}^n, s} \max_{q>0} L(q,y,s) \tag{3.4}$$

At optimality the gradient of the Lagrangian is zero, so for any κ,

$$\partial_{q_\kappa} L(q,y,s) = 0 \Leftrightarrow \log\frac{c_p(\kappa)}{q_\kappa} - 1 = -\sum_{i=1}^n y_i\kappa_i = -\langle y,\kappa\rangle - s.$$

Therefore, at optimality

$$\frac{c_p(\kappa)}{q_\kappa} = e^{1-\langle y,\kappa\rangle - s}.$$

Plugging this into (3.4), we can write the dual as follows:

$$\inf_{y,s} \sum_{\kappa\in\mathrm{Newt}(p)} q_\kappa(1-\langle y,\kappa\rangle - s) - \langle y,\alpha\rangle + \sum_{i=1}^n y_i \sum_{\kappa\in\mathrm{Newt}(p)} q_\kappa \kappa_i - s + s\sum_{\kappa\in\mathrm{Newt}(p)} q_\kappa \tag{3.5}$$

$$= \inf_{y,s} \sum_{\kappa\in\mathrm{Newt}(p)} q_\kappa - \langle y,\alpha\rangle - s \tag{3.6}$$

$$= \inf_{y,s} \sum_{\kappa\in\mathrm{Newt}(p)} c_p(\kappa) e^{s+\langle y,\kappa\rangle-1} - \langle y,\alpha\rangle - s \tag{3.7}$$

Optimizing the RHS over s we get

$$1 = \sum_{\kappa\in\mathrm{Newt}(p)} c_p(\kappa) e^{s+\langle y,\kappa\rangle-1} \Leftrightarrow s = -\log \sum_{\kappa\in\mathrm{Newt}(p)} c_p(\kappa) e^{\langle y,\kappa\rangle-1}$$

Plugging in the value of s, we can rewrite the dual as follows:

$$\inf_y 1 - \langle y,\alpha\rangle + \log \sum_{\kappa\in\mathrm{Newt}(p)} c_p(\kappa) e^{\langle y,\kappa\rangle-1} = \inf_y \log \frac{p(e^{y_1},\dots,e^{y_n})}{y^\alpha}$$

as desired.

3.2 Applications to TSP

Recall that in the traveling salesperson problem (TSP) we are given a list of n cities $\{1,\dots,n\}$ and their symmetric pairwise distances, $c:[n]\times[n]\to\mathbb{R}_+$ that satisfies the triangle inequality, $c(i,j)\le c(i,k)+c(k,j)$ for all distinct triplet of vertices $1\le i,j,k\le n$. We want to find the shortest tour that visits each vertex exactly once. Consider the LP relaxation of TSP

$$\begin{aligned} \max \quad & \sum_{i,j} c(i,j) x_{\{i,j\}}, & \\ \text{s.t.,} \quad & \sum_{i\in S, j\notin S} x_{\{i,j\}} \ge 2 & \forall S \subsetneq V \\ & \sum_j x_{\{i,j\}} = 2 & \forall i, \\ & x_{\{i,j\}} \ge 0 & \forall i,j. \end{aligned} \tag{3.8}$$

Let x^0 be an optimal solution. It turns out that without loss of generality we can assume that there exists an edge e_0 such that $x^0_{e_0} = 1$ and $c(e_0) = 0$. Without loss of generality, assume $e_0 = (n-1,n)$. We let E_0 be the support of x^0, i.e., set $\{i,j\}$ where $x_{\{i,j\}} > 0$. Let $E = E_0 \smallsetminus \{e_0\}$ and $G = (V,E)$. Let x be x^0 restricted to E. It turns out that the vector x is in the spanning tree polytope of G. Note that every vertex (except $n-1,n$) has fractional degree exactly 2 in x, i.e., for any $i < n-1$, $\sum_{e\sim i} x_e = 2$ and $n-1,n$ have (fractional) degree 1.

Let μ be the uniform distribution over spanning trees of $G=(V,E)$. By Theorem 3.2, there exists an external field λ such that marginals of $\mu * \lambda$ is equal to α. We use the following maximum entropy algorithm for TSP: Sample $T \sim \mu * \lambda$. Let M be the the minimum cost matching on odd degree vertices of T. Return $T \cup M$; we can turn $T \cup M$ to a Hamiltonian cycle by taking an Eulerian tour and "shortcutting" every second time that we visit a vertex.

Very recently, in a joint work with Anna Karlin and Nathan Klein we proved the following theorem:

Theorem 3.4 ([KKO20])**.** *For some $\epsilon \geq 10^{-36}$, the maximum entropy algorithm gives a $1.5-\epsilon$ approximation algorithm for TSP.*

The proof uses many properties of Strongly Rayleigh distribution $\mu * \lambda$.

Next, we will explain a crucial property of such a distribution and the generalization which is used in our work.

Lemma 3.5. *Let $v_1, \dots, v_k$ be vertices of G that do not include $n-1, n$ such that the induced graph $G[\{v_1, \dots, v_k\}]$ has no edges. Then,*

$$\mathbb{P}_{T \sim \mu * \lambda}\left[d_T(v_1) = \cdots = d_T(v_k) = 2\right] \geq e^{-k}$$

where $d_T(v)$ is the degree of a vertex v in the sampled tree T.

Proof. Let $S_1, \dots, S_k$ be the set of edges incident to $v_1, \dots, v_k$ respectively and let F be the rest of the edges. Note that since $v_1, \dots, v_k$ do not share edges, $S_1, \dots, S_k$ are mutually disjoint. Define

$$p(y_1, \dots, y_k) = g_{\mu*\lambda}\left(\begin{cases} z_e = y_1 & \forall e \in S_1, \\ \dots & \\ z_e = y_k & \forall e \in S_k \\ z_e = 1 & \text{otherwise} \end{cases}\right).$$

Note that in this definition we crucially use that $S_1, \dots, S_k$ are disjoint. By closure properties of real stable polynomials p is real stable. We can re-write p as follows:

$$p(y_1, \dots, y_k) = \sum_T \mu * \lambda(T) \prod_{i=1}^k y_i^{d_T(v_i)}.$$

It follows that

$$\mathbb{P}\left[d_T(v_1) = \cdots = d_T(v_k) = 2\right] = 2^{-k} \partial_{y_1}^2 \dots \partial_{y_k}^2 p|_{y=0},$$

i.e., the RHS is the coefficient of $y_1^2 \dots y_k^2$ in p. Furthermore, note that each of the vertices $v_1, \dots, v_k$ have degree at least 1 in T; so we can factor out a monomial $y_1 \dots y_k$,

$$p(y) = y_1 \dots y_k q(y_1, \dots, y_k).$$

It follows that q is also real stable. So, we need to show that

$$\partial_{y_1} \dots \partial_{y_k} q|_{y=0} \geq e^{-k}.$$

Since q is real stable and has non-negative coefficients, by Gurvits' Theorem 2.3, we have

$$\partial_{y_1} \dots \partial_{y_k} q|_{y=0} \geq e^{-k} \inf_{y>0} \frac{q(y)}{y_1 \dots y_k}.$$

So, all we need to show is that

$$\inf_{y>0} \frac{q(y)}{y_1 \dots y_k} \geq 1. \tag{3.9}$$

First, observe that we can write q as follows:

$$\begin{aligned} q(y_1,\dots,y_k) &= \sum_T \mu * \lambda(T) \prod_{i=1}^k y_i^{d_T(v_i)-1} \\ &\geq \prod_T \left(\prod_{i=1}^k y_i^{d_T(v_i)-1}\right)^{\mu*\lambda(T)} \\ &= \prod_{i=1}^k y_i^{\sum_T \mu*\lambda(T) d_T(v_i)-1} = \prod_{i=1}^k y_i^{2-1}, \end{aligned}$$

where the inequality follows by weighted AM-GM and the last identity follows by the fact that $\mathbb{E}\left[d_T(v)\right] = 2$ for any vertex other than $n-1, n$. This proves (3.9). □

We proved the following generalization of the above fact in [KKO20].

Theorem 3.6. *Given a SR distribution $\mu : 2^{[n]} \to \mathbb{R}_+$, and disjoint sets $A_1, \dots, A_k$ such that for any $S \subseteq [k]$,*

$$\mathbb{P}_{T\sim\mu}\left[\sum_{i\in S} |T \cap A_i| = |S|\right] \geq \epsilon$$

Then,

$$\mathbb{P}\left[\forall i : |T \cap A_i| = 1\right] \geq \frac{\epsilon^{2^k+1}}{k!}.$$

In the exercises we will see the proof of the above theorem for $k = 2$. See a recent work of Gurvits and Leake [GL20] for a somewhat stronger bound.

References

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