A Bound on the Sum of Weighted Pairwise Distances of Points Constrained to Balls *

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Abstract

We consider the problem of choosing Euclidean points to maximize the sum of their weighted pairwise distances, when each point is constrained to a ball centered at the origin. We derive a dual minimization problem and show strong duality holds (i.e., the resulting upper bound is tight) when some locally optimal configuration of points is affinely independent. We sketch a polynomial time algorithm for finding a near-optimal set of points.

1 Introduction

We consider the following maximization problem $P(n, w, \ell)$:

$$\text{maximize}_{\{p_i\}} \sum_{1\le i<j\le n} w(i,j)d(p_i,p_j)$$

$$\text{subject to} \begin{cases} p_i \in \mathbb{R}^{n-1} & (i=1,..,n); \\ ||p_i|| \le \ell(i) & (i=1,..,n). \end{cases}$$

Here each $w(i,j) \ge 0$ and each $\ell(i) \ge 0$ is fixed, $d(p,q)$ denotes the Euclidean distance between points p and q, and $||p||$ denotes the Euclidean length (distance from the origin) of point p.

We derive the following dual problem $D(n, w, \ell)$:

$$\text{minimize}_{\{x_i\}} \sqrt{\sum_{1\le i<j\le n} \frac{w^2(i,j)}{x_i x_j}} \times \sqrt{\sum_{i=1}^n \ell^2(i) x_i} \times \sqrt{\sum_{i=1}^n x_i}$$

$$\text{subject to} \begin{cases} x_i \in \mathbb{R} & (i=1,..,n); \\ x_i \ge 0 & (i=1,..,n). \end{cases}$$

Throughout the paper, $\frac{0}{0}$ is defined to be 0.

We show that the value of the maximization problem is at most the value of the minimization problem. We use a physical interpretation of the two problems to show that the values are equal

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provided the maximization problem admits a set of points $\{p_i\}$ that is both affinely independent and stationary (i.e., the gradient of the objective function is a nonnegative combination of the gradients of the active constraints, a necessary condition at any local maximizer of $P(n, w, \ell)$).

We sketch how a near-optimal solution to the problem can be found in polynomial time via the ellipsoid method.

2 Related Work

The case $w(i,j) = \ell(i) = 1$ (in which the optimal points are given by the vertices of the regular n-simplex, achieving a value of $n\sqrt{\binom{n}{2}}$) was previously considered by [3]. Our Lemma 1 generalizes a bound in that paper.

Specific instances of $P(n, w, \ell)$ were studied to obtain geometric inequalities that were used to analyze approximation algorithms for finding low-degree, low-weight spanning trees in Euclidean spaces [2].

Goemans and Williamson [1] consider related problems with applications to approximating the maximum cut in a graph and to maximizing the number of satisfied clauses in a CNF formula. We modify their approach to solving their problems to obtain a polynomial time algorithm for ours.

3 A Dual Problem

Lemma 1 *For any n, w, and ℓ, the value of the maximization problem $P(n, w, \ell)$ is at most the value of the minimization problem $D(n, w, \ell)$.*

Proof: Fix any n, w, and ℓ. Fix any set of points $\{p_i\}$ and values $\{x_i\}$ meeting the constraints of $P(n, w, \ell)$ and $D(n, w, \ell)$, respectively. Let $A(i,j) = \frac{w(i,j)}{\sqrt{x_i x_j}}$ and $B(i,j) = \sqrt{x_i x_j}\, d(p_i, p_j)$ for $1 \le i < j \le n$. Then, by the Cauchy-Schwartz inequality $A \cdot B \le \|A\| \times \|B\|$ (where A and B are interpreted as $\binom{n}{2}$-dimensional vectors, and $\cdot$ denotes the dot product):

$$\sum_{i<j} w(i,j) d(p_i, p_j) \le \sqrt{\sum_{i<j} \frac{w^2(i,j)}{x_i x_j}} \times \sqrt{\sum_{i<j} x_i x_j d^2(p_i, p_j)}. \tag{1}$$

It remains only to show

$$\sum_{i<j} x_i x_j d^2(p_i, p_j) \le \left(\sum_i x_i\right) \times \left(\sum_i \ell^2(i) x_i\right).$$

Expanding the left-hand side,

$$\begin{aligned}
&\sum_{i<j} x_i x_j d^2(p_i, p_j) \\
&= \frac{1}{2} \sum_{i,j} x_i x_j (p_i - p_j) \cdot (p_i - p_j) \\
&= \frac{1}{2} \sum_{i,j} x_i x_j (p_i \cdot p_i - 2 p_i \cdot p_j + p_j \cdot p_j)
\end{aligned}$$

$$
\begin{aligned}
&\le \sum_{i,j} x_i x_j(\ell^2(i) - p_i \cdot p_j) && (2)\\
&= \left(\sum_i x_i\right) \times \left(\sum_i x_i \ell^2(i)\right) - \left(\sum_i x_i p_i\right) \cdot \left(\sum_i x_i p_i\right)\\
&= \left(\sum_i x_i\right) \times \left(\sum_i x_i \ell^2(i)\right) - \left\|\sum_i x_i p_i\right\|^2\\
&\le \left(\sum_i x_i\right) \times \left(\sum_i x_i \ell^2(i)\right). && (3)
\end{aligned}
$$

□

Lemma 2 *Fix any n, w, and ℓ. Suppose the maximization problem $P(n, w, \ell)$ admits a set of points $\{p_i\}$ that is both stationary and affinely independent. Then the values of the two problems are equal. Further, there exists $\{x_i\}$ such that*

$$
x_i p_i = \sum_j w(i,j) \frac{p_i - p_j}{d(p_i, p_j)} \tag{4}
$$

(where $x_i = 0$ in case $\|p_i\| < \ell_i$, and $w(i,j) = w(j,i)$ and $w(i,i) = 0$), and $\{p_i\}$ and $\{x_i\}$ are global optima for the two problems.

Proof: Fix any n, w, and ℓ. Consider the objective function $\Phi(\{p_i\}) = \sum_{ij} w(i,j) d(p_i, p_j)$ of $P(n, w, \ell)$. That $\{p_i\}$ is stationary means that the gradient of Φ is a nonnegative combination of the gradients of the constraints of $P(n, w, \ell)$ active at $\{p_i\}$. By elementary calculus, the gradient of Φ consists of a vector f_i for each point p_i, with each f_i equal to the right-hand side of (4). The only constraint on p_i is $\|p_i\| \le \ell(i)$, whose gradient (again by elementary calculus) is a nonnegative multiple of p_i. Thus, for each i, there exists an $x_i \ge 0$ such that (4) holds. Note that if $\|p_i\| < \ell(i)$, then the constraint is not active, so that f_i must be the zero vector. In this case we take $x_i = 0$.

We will show that each inequality in Lemma 1 is tight for these $\{p_i\}$ and $\{x_i\}$. Inequality (3) is tight because, by (4), $\sum_i x_i p_i$ is the zero vector. Inequality (2) is tight because $\|p_i\| < \ell(i)$ only if $x_i = 0$.

Inequality (1) is tight provided the vector A (in the proof of Lemma 1) is a scalar multiple of B. Assume $\{p_i\}$ is affinely independent. Then, considering $\{x_i\}$ and $\{p_i\}$ fixed and $\{w(i,j)\}$ as the set of unknowns (i.e., reversing their roles), (4) uniquely determines each $w(i,j)$. Since

$$
w(i,j) = \frac{x_i x_j d(p_i, p_j)}{\sum_k x_k} \quad (1 \le i < j \le n) \tag{5}
$$

is consistent with (4) (check this by substitution for $w(i,j)$ in (4)), it follows that (5) necessarily holds. Thus, A is a scalar multiple of B and Inequality (1) is tight. □

A physical model for the quantities involved is as follows. Consider a physical system of n points $\{p_i\}$. Each point p_i is constrained to a ball of radius $\ell(i)$ centered at the origin. For each pair of points (p_i, p_j), p_i repels p_j (and vice versa) with a force of magnitude $w(i,j)$.

Under this interpretation, each vector f_i in the proof corresponds to the force on p_i, and x_i is the magnitude of this force, divided by $\|p_i\|$.

4 Solving $P(n, w, \ell)$ in Polynomial Time

If the instance of $P(n, w, \ell)$ is small or has a high degree of symmetry, the dual problem $D(n, w, \ell)$ might yield a function that can be minimized directly by symbolic methods. In general, it is possible to solve $P(n, w, \ell)$ (to any given degree of precision) in polynomial time using semi-definite programming, following the approach in [1].

Those authors consider a related problem $GW(w, n)$:

$$\text{maximize}_{\{p_i\}} \sum_{1 \le i < j \le n} w(i,j) d^2(p_i, p_j)$$

$$\text{subject to} \begin{cases} p_i \in \mathbb{R}^n & (i = 1, .., n); \\ \|p_i\| = 1 & (i = 1, .., n). \end{cases}$$

The authors show how to solve this problem in polynomial time by formulating it as a semi-definite program, and how to round a (near-)optimal set of points $\{p_i\}$ to obtain an approximate solution to a corresponding max-cut problem. This approach yielded the first polynomial-time approximation algorithm achieving a performance guarantee better than two for the max-cut problem.

We briefly sketch their aproach for solving $GW(w, n)$ and how it can be modified to solve $P(w, n, \ell)$. The connection between sets of points and positive semi-definite matrices is the following: an $n \times n$ symmetric matrix Y is positive semi-definite if and only if there exists a set of n points $\{p_i\}$ in $\mathbb{R}^n$ such that $Y_{ij} = p_i \cdot p_j$. Thus, $GW(w, n)$ is equivalent to following:

$$\text{maximize}_{\{Y\}} \sum_{ij} w(i,j)(2 - 2Y_{ij})$$

$$\text{subject to} \begin{cases} Y \text{ is an } n \times n \text{ symmetric, positive semi-definite matrix;} & \\ Y_{ii} = 1 & (i = 1, .., n). \end{cases}$$

The space of $n \times n$ symmetric, positive semi-definite matrices admits a polynomial time separation oracle because a symmetric matrix Y is positive semi-definite if and only if $x^T Y x \ge 0$ for each $x \in \mathbb{R}^n$, and in fact it suffices to check each eigenvector x of Y. Thus, combining the constraint that Y is positive semi-definite with arbitrary linear inequalities on the elements of Y yields a convex space with a polynomial time separation oracle. Approximate feasibility of such a problem is testable in polynomial time via the ellipsoid method. Thus, $GW(n)$ can be solved to near-optimality in polynomial time.

A similar approach can be used to solve $P(n, w, \ell)$ in polynomial time. In particular, $P(n, w, \ell)$ corresponds to the following semi-definite program:

$$\text{maximize}_{\{Y\}} \sum_{ij} w(i,j) \sqrt{Y_{ii} + Y_{jj} - 2Y_{ij}}$$

$$\text{subject to} \begin{cases} Y \text{ is an } n \times n \text{ symmetric, positive semi-definite matrix;} & \\ Y_{ii} \le \ell(i) & (i = 1, .., n). \end{cases}$$

Since $\sum_{ij} w(i,j) \sqrt{Y_{ii} + Y_{jj} - 2Y_{ij}}$ is a concave function in $\{Y_{ij}\}$ whose gradient can be computed in polynomial time, the above program also admits a separation oracle sufficient to solve it to near-optimality in polynomial time using the ellipsoid method.

5 Open Problems

It would be interesting to obtain a more efficient algorithm for solving $P(w, n, \ell)$ than is obtained by reducing to the ellipsoid method. Especially interesting would be a primal-dual algorithm along the lines of traditional "combinatorial" algorithms for solving or approximating linear programs. It is not clear how to achieve such algorithms in the semi-definite setting.

Similarly, the only known method for achieving a better factor than two for the max-cut problem is by reduction to semi-definite programming. Goemans and Williamson leave open the problem of finding a more efficient algorithm that beats a factor of two. A more efficient algorithm for $P(n, w, \ell)$ (with each $\ell(i) = 1$) would solve this, because applying their randomized rounding technique to $P(n, w, \ell)$ also yields an approximation algorithm for max-cut with performance guarantee better than two.

On the other hand, consider the generalization of $GW(n, w)$ in which the objective function is replaced by $\sum_{ij} w(i, j)d^{2+\epsilon}(p_i, p_j)$ for some $\epsilon \geq 0$. For $\epsilon > 0$, applying Goemans and Williamson's approach to this program rather than $GW(n, w)$ would provide a better approximation to max-cut. Is the generalization solvable in polynomial time for some $\epsilon > 0$?

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References

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