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 $P(n, w, \ell)$:

$$\text{maximize} \left\{ \sum_{1 \leq i < j \leq n} w(i, j)d(p_i, p_j) \right\} \quad \text{subject to} \quad \begin{cases} p_i \in \mathbb{R}^{n-1} & (i = 1, \ldots, n); \\ ||p_i|| \leq \ell(i) & (i = 1, \ldots, n). \end{cases}$$

Here each $w(i, j) \geq 0$ and each $\ell(i) \geq 0$ 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 $D(n, w, \ell)$:

$$\text{minimize} \left\{ \sum_{1 \leq i < j \leq n} \frac{w^2(i, j)}{x_i x_j} \times \sum_{i=1}^{n} \ell^2(i) x_i \times \sqrt{\sum_{i=1}^{n} x_i} \right\} \quad \text{subject to} \quad \begin{cases} x_i \in \mathbb{R} & (i = 1, \ldots, n); \\ x_i \geq 0 & (i = 1, \ldots, n). \end{cases}$$

Throughout the paper, $0 \times 0$ 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 \( \ell \), 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 \( \ell \). 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 \( 1 \leq i < j \leq n \). Then, by the Cauchy-Schwartz inequality \( A \cdot B \leq \|A\| \times \|B\| \) (where \( A \) and \( B \) are interpreted as \( \binom{n}{2} \)-dimensional vectors, and \( \cdot \) denotes the dot product):

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

It remains only to show

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

Expanding the left-hand side,

\[
\sum_{i < j} x_i x_j d^2(p_i, p_j)
= \frac{1}{2} \sum_{i, j} x_i x_j (p_i - p_j) \cdot (p_i - p_j)
= \frac{1}{2} \sum_{i, j} x_i x_j (p_i \cdot p_i - 2p_i \cdot p_j + p_j \cdot p_j)
\]
\[
\leq \sum_{i,j} x_i x_j (\ell^2(i) - p_i \cdot p_j)
\]
(2)

\[
= \left( \sum_i x_i \right) \times \left( \sum_i x_i \ell^2(i) \right) - \left( \sum_i x_i p_i \right) \cdot \left( \sum_i x_i p_i \right)
\]
(3)

\[
= \left( \sum_i x_i \right) \times \left( \sum_i x_i \ell^2(i) \right) - \left( \sum_i x_i p_i \right)^2
\]

\[
\leq \left( \sum_i x_i \right) \times \left( \sum_i x_i \ell^2(i) \right).
\]

Lemma 2  Fix any \(n, w, \) and \(\ell\). 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

\[
x_i p_i = \sum_j w(i, j) \frac{p_i - p_j}{d(p_i, p_j)}
\]
(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 \(\ell\). 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 \(\Phi\) 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 \(\Phi\) 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 \(\|p_i\| \leq \ell(i)\), whose gradient (again by elementary calculus) is a nonnegative multiple of \(p_i\). Thus, for each \(i\), there exists an \(x_i \geq 0\) 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

\[
w(i, j) = \frac{x_i x_j d(p_i, p_j)}{\sum_k x_k} \quad (1 \leq i < j \leq n)
\]
(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 $GW(w, n)$:

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

subject to

$$p_i \in \mathbb{R}^n (i = 1, \ldots, n);$$

$$\|p_i\| = 1 (i = 1, \ldots, n).$$

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 approach 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:

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

subject to

$$Y$$

is an $n \times n$ symmetric, positive semi-definite matrix;

$$Y_{ii} = 1 (i = 1, \ldots, n).$$

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 $x^T Y x \geq 0$ 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:

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

subject to

$$Y$$

is an $n \times n$ symmetric, positive semi-definite matrix;

$$Y_{ii} \leq \ell(i) (i = 1, \ldots, n).$$

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

[1] Michel Goemans and David Williamson. .878-approximation algorithms for MAX CUT and MAX 2SAT. In Proc. of the 26th Ann. ACM Symp. on Theory of Computing, 1994.

[2] Samir Khuller, Balaji Raghavachari, and Neal Young. Low-degree spanning trees of small weight. In Proc. of the 26th Ann. ACM Symp. on Theory of Computing, 1994.

[3] J. N. Lillington. Some extremal properties of convex sets. Math. Proc. Cambridge Philosophical Society, 77:515–524, 1975.