Clustering with Iterated Linear Optimization

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Abstract

We introduce a novel method for clustering using a semidefinite programming (SDP) relaxation of the Max $k$-Cut problem. The approach is based on a new methodology for rounding the solution of an SDP using iterated linear optimization. We show the vertices of the Max $k$-Cut SDP relaxation correspond to partitions of the data into at most $k$ sets. We also show the vertices are attractive fixed points of iterated linear optimization. We interpret the process of fixed point iteration with linear optimization as repeated relaxations of the closest vertex problem. Our experiments show that using fixed point iteration for rounding the Max $k$-Cut SDP relaxation leads to significantly better results when compared to randomized rounding.

1 Introduction

Semidefinite programming (SDP) relaxations have led to significant advances in the development of combinatorial optimization algorithms. Many challenging optimization problems can be approximately solved by a combination of an SDP relaxation and a rounding step. One of the best examples of this paradigm is the celebrated Max Cut algorithm of Goemans and Williamson [10].

From a theoretical point of view algorithms based on SDP relaxations can lead to strong approximation guarantees. However, such approximation guarantees do not always translate to practical solutions. Many algorithms with good theoretical guarantees rely on randomized rounding methods that can produce solutions that have undesirable artifacts despite having relatively high objective value. This motivates the development of effective deterministic methods for rounding the solutions of SDP relaxations. Recent advances based on the sum-of-squares hierarchy have also motivated the development of new general methods for rounding the solutions of SDP relaxations [3].

In this paper we introduce a novel method for clustering using the Max $k$-Cut SDP relaxation described in [9]. The approach is based on a new methodology for rounding the solution of an SDP relaxation introduced by the current authors in a recent paper [8]. Our rounding method involves fixed point iteration with a map that optimizes a linear function over a convex body. Figure 1 shows an example comparing the result of our fixed point iteration method for rounding the solution of the Max $k$-Cut SDP relaxation to the result obtained using randomized rounding.

As pointed out already by the authors of [9], the randomized rounding method has some significant shortcomings. The approximation factor of the randomized algorithm appears good on the surface, but is not much better from the approximation factor one gets by randomly partitioning the data. Randomized rounding often actually generates a partition with fewer than $k$ sets. The result in Figure 1(b) is a partition with 7 non-empty clusters despite the fact that $k = 8$. We also see in Figure 1(b) that the resulting clusters are not compact. Instead different clusters have significant overlap. In Section 6 we compare our fixed point iteration method to the randomized rounding.
Figure 1: Clustering 120 points into 8 clusters: (a) input data, (b) clustering using randomized rounding, and (c) clustering using fixed point iteration. Each cluster is shown with a different color and a minimal enclosing circle. A solution to the Max $k$-Cut SDP relaxation is a matrix in the $k$-way elliptope. (d) illustrates the sequence of matrices obtained by fixed point iteration starting from the SDP solution. The final matrix is an integer solution defining a clustering.
rounding procedure in several examples, showing that the fixed point approach can produce much better clusterings in practice.

The work in [16] gives a general method for derandomizing approximation algorithms based on SDP relaxations, including the Max k-Cut relaxation we use for clustering. Although the method in [16] is interesting from a theoretical point of view, the approach is not practical for problems of non-trivial size. More recent methods for derandomizing the Max Cut approximation algorithm include [7] and [4]. These methods are all based on the randomized rounding method of [10] but replace the randomization with a search over a limited number of discretized choices. In contrast, our fixed point iteration method is not based on derandomization techniques and is instead based on a novel approach for rounding the solution of an SDP relaxation.

The SDP relaxation for Max k-Cut involves linear optimization in a convex body that we call the k-way ellipotope. In Section 4 we show that the vertices of the k-way ellipotope correspond to partitions (clusterings) of the data into at most k sets, generalizing the result from [13] for the ellipotope (the k = 2 case).

In a companion paper ([8]) we showed that iterated linear optimization in a convex region always converges to a fixed point. In the case of the k-way ellipotope the resulting fixed point corresponds to an integer solution to the Max k-Cut problem and defines a partitioning of the data. Intuitively the problem of rounding a solution of the SDP relaxation can be interpreted as a new clustering problem that can be solved recursively.

For some applications convex relaxations have been shown to recover the “true” hidden structure in the data (see, e.g., [5]). For clustering applications it was shown in [2] that convex relaxations can recover a ground truth clustering if the data is sufficiently well-separated. However, in practice the data is rarely well-separated (and there is often no ground truth clustering). Nonetheless, good clusterings might exist that can be extremely useful for data processing, coding or analysis. The data in Figure 1 illustrates an example of this situation. The data was generated by sampling from several Gaussian distributions with significant overlap. In this case there is no way to recover the ground truth clustering, but the result of our fixed point iteration method still provides a good solution that can be used for subsequent analysis.

In Section 2 we discuss how Max k-Cut can be used to formulate the clustering problem. In Section 3 we review the Max k-Cut SDP relaxation and the randomized rounding method from [9]. In Section 4 we study the convex body that arises from the SDP relaxation and show the vertices of the feasible region correspond to partitions. In Section 5 we describe how iterated linear optimization leads to a deterministic method for rounding the solution of the SDP relaxation. Finally, in Section 6 we illustrate experimental results of our new rounding method and compare them to the randomized rounding approach from [9].

2 Clustering with Max k-Cut

Clustering problems are often formulated using pairwise measures of similarity or dissimilarity between data points. Intuitively we would like to partition the data so that pairs of points within a cluster are similar to each other while pairs of points in different clusters are dissimilar. This idea leads to a variety of formulations of clustering as graph partition problems.

Let $G = (V, E)$ be a weighted graph. Let $[n] = \{1, \ldots, n\}$. To simplify notation we assume throughout that $V = [n]$ and that the graph is complete. A k-partition is a partition of $V$ into $k$ disjoint sets $(A_1, \ldots, A_k)$, some of which may be empty. Let $M$ be a symmetric matrix of pairwise
non-negative weights. The weight of a partition \( P \) is the sum of the weights of the pairs \( \{i, j\} \subseteq [n] \) that are split (or cut) by \( P \),

\[
w(P) = \sum_{1 \leq r < s \leq k} \sum_{i \in A_r} \sum_{j \in A_s} M_{i,j}.
\]

The Max \( k \)-Cut problem is to find a \( k \)-partition maximizing \( w(P) \).

As an example, let \( D = \{x_1, \ldots, x_n\} \) be \( n \) points in \( \mathbb{R}^d \). One of the most commonly used formulations for clustering data in Euclidean space involves optimizing the \( k \)-means objective. For \( A \subseteq [n] \) let \( m(A) \) be the mean of the points indexed by \( A \),

\[
m(A) = \frac{1}{|A|} \sum_{i \in A} x_i.
\]

The \( k \)-means objective (1) is to partition the data into clusters to minimize the sum of squared distances from each point to the center of its cluster,

\[
\argmin_{(A_1, \ldots, A_k)} \sum_{r=1}^{k} \sum_{i \in A_r} ||x_i - m(A_i)||^2.
\]

This objective encourages partitions of the data into “compact” clusters, and is widely used both for clustering and for vector quantization in coding applications (see, e.g., [14, 15, 11, 1]).

Let \( M_{i,j} = ||x_i - x_j||^2 \). Maximizing the weight of the pairs \( \{i, j\} \) that are split by a partition is the same as minimizing the weights of the pairs \( \{i, j\} \) that are not split. Moreover, the sum of squared distances between points within a set \( A_i \) can be expressed in terms of the sum of squared distances between each point in \( A_i \) and the mean of the set:

\[
\argmax_{(A_1, \ldots, A_k)} w(A_1, \ldots, A_k) = \argmin_{(A_1, \ldots, A_k)} \sum_{r=1}^{k} \sum_{i,j \in A_r} ||x_i - x_j||^2,
\]

\[
= \argmin_{(A_1, \ldots, A_k)} \sum_{r=1}^{k} |A_r| \sum_{i \in A_r} ||x_i - m(A_r)||^2.
\]

The objective function (3) is similar to the \( k \)-means objective (1), except that in the case of Max \( k \)-Cut there is a preference towards balanced partitions. In Section 6 we illustrate the results of clustering experiments with Max \( k \)-Cut using this formulation.

The work in [21] also considered clustering with Max \( k \)-Cut and used an SDP relaxation together with randomized rounding to solve the resulting problem. That work focused on an information theoretical formulation of the clustering problem that could also be used within our framework.

Most of the previous work on clustering using graph-based methods has focused on formulations based on minimum cuts and spectral algorithms ([20, 17, 18, 22, 12]). In this case the weight of an edge represents similarity (or affinity) between elements instead of dissimilarity. Minimum cut formulations often include some form of normalization (see, e.g., [20, 12]) or a balance requirement to avoid trivial partitions (otherwise the cut is minimized when one partition is very small). In contrast to minimum cut formulations, clustering using a maximum cut formulation naturally encourages balanced partitions, as they maximize the total number of edges that are split.
3 SDP Relaxation for Max k-Cut

The Goemans and Williamson approximation algorithm for Max Cut (clustering into two clusters) is based on an SDP relaxation and a randomized rounding method [10]. The relaxation involves the optimization of a linear function over a convex body $L_n$ known as the elliptope. Laurent and Poljak [13] showed that the vertices of $L_n$ correspond to bipartitions of $[n]$. The fact that the vertices of $L_n$ are bipartitions gives an explanation as to why in some cases the SDP relaxation can lead directly to an integer solution defining an optimal solution to the Max Cut problem (see also [6]).

Frieze and Jerrum [9] generalized the Max Cut algorithm of Goemans and Williamson to a randomized approximation method for Max $k$-Cut. In this case the algorithm involves linear optimization over a convex body $L_{n,k}$ that we call the $k$-way elliptope.

Below we briefly review the relaxation and randomized approximation algorithm for Max $k$-Cut. In Section 4 we show the vertices of the $k$-way elliptope correspond to $k$-partitions, generalizing the result from [13] for the elliptope. In Section 5 we describe a determinisic method for rounding the solution of the SDP relaxation for Max $k$-Cut based on iterated linear optimization.

The Max $k$-Cut relaxation is based on a reformulation of the combinatorial problem in terms of Gram matrices. Let $a_1, \ldots, a_k$ be the vertices of an equilateral simplex $\Sigma_k$ in $\mathbb{R}^{k-1}$ centered around the origin and scaled such that $||a_i|| = 1$. For $i \neq j$ we have $a_i \cdot a_j = -1/(k-1)$.

A $k$-partition $P = (A_1, \ldots, A_k)$ can be encoded by $n$ vectors $(y_1, \ldots, y_n)$ with $y_i = a_j$ if $i \in A_j$. Define the $k$-partition matrix $X^P$ to be the Gram matrix of $(y_1, \ldots, y_n)$. Then

$$X^P_{i,j} = \begin{cases} 1 & \text{if } \{i, j\} \text{ are together in } P \\ -1/(k-1) & \text{if } \{i, j\} \text{ are split by } P \end{cases}$$

$$1 - X^P_{i,j} = \begin{cases} 0 & \text{if } \{i, j\} \text{ are together in } P \\ k/(k-1) & \text{if } \{i, j\} \text{ are split by } P \end{cases}$$

Using this relation the weight of a partition, $w(P)$, can be written as,

$$w(P) = \frac{k-1}{2k} (1 - X^P) \cdot M,$$

where $M$ is the symmetric matrix of pairwise weights.

Definition 1. The set of $k$-partition matrices $Q_{n,k}$ is the set of Gram matrices of $n$ vectors $(y_1, \ldots, y_n)$ with $y_i \in \{a_1, \ldots, a_k\}$ for $1 \leq i \leq n$.

We can reformulate the Max $k$-Cut problem as an optimization over $k$-partiton matrices,

$$\arg\max_{X \in Q_{n,k}} \frac{k-1}{2k} (1 - X) \cdot M.$$
The matrices in $L_n$ exactly correspond to Gram matrices of $n$ unit vectors $(y_1,\ldots,y_n)$ in $\mathbb{R}^n$ (10 13).

**Definition 3.** The $k$-way elliptope $L_{n,k}$ is the subset of matrices in $L_n$ where every entry is at least $-1/(k-1)$:

$$L_{n,k} = \{X \in L_n | X_{i,j} \geq -1/(k-1)\}.$$ 

The matrices in $L_{n,k}$ correspond to Gram matrices of $n$ unit vectors $(y_1,\ldots,y_n)$ in $\mathbb{R}^n$ with $v_i \cdot v_j \geq -1/(k-1)$.

The algorithm in [9] involves the SDP relaxation,

$$\argmax_{X \in L_{n,k}} \frac{k-1}{2k} (1 - X) \cdot M.$$ 

Let $X$ be the solution of the SDP relaxation. We can interpret $X$ as the Gram matrix of $n$ unit vectors $(y_1,\ldots,y_n)$ in $\mathbb{R}^n$, obtained using a Cholesky decomposition $X = VV^T$. To generate a $k$-partition the randomized method selects $k$ unit vectors $(u_1,\ldots,u_k)$ independently at random from a uniform distribution and assigns $y_i$ to the closest vector $u_j$.

When $k > 2$ rounding a $k$-partition matrix $X^P$ using the randomized procedure above can generate a partition that is different from $P$ because different sets in $P$ can be merged. More generally the random rounding procedure often generates a partition with fewer than $k$ sets because some vector $u_j$ is not the closest vector to any $v_i$. In Section 6 we show experimental results that illustrate several problems that arise in practice when using the randomized rounding procedure. Even when the cut value of the random partition is relatively high, the resulting clustering can have undesirable artifacts.

### 4 The $k$-way elliptope

The main result of this section is that the vertices of $L_{n,k}$ are the matrices in $Q_{n,k}$ and correspond to $k$-partitions of $[n]$. Note that a $k$-partition may have some empty sets, so the vertices of $L_{n,k}$ correspond to partitions of $[n]$ into at most $k$ sets.

For a matrix $X \in S_3$ we have

$$X = \begin{pmatrix} 1 & x & y \\ x & 1 & z \\ y & z & 1 \end{pmatrix}.$$ 

Therefore we can visualize $X$ as a point $(x,y,z) \in \mathbb{R}^3$.

Figure 2 illustrates $L_{3,2}$ (the elliptope). This convex body has 4 vertices, with one vertex for each partition of 3 distinguished elements into at most 2 sets. The partitions are listed below.

- $P_1 = (\{1,2,3\},\emptyset)$
- $P_2 = (\{1,2\},\{3\})$
- $P_3 = (\{1,3\},\{2\})$
- $P_4 = (\{2,3\},\{1\})$

Figure 3 illustrates $L_{3,3}$. This convex body has 5 vertices, with one vertex for each partition of 3 distinguished elements into at most 3 sets. The partitions are listed below.

- $P_1 = (\{1,2,3\},\emptyset,\emptyset)$
- $P_2 = (\{1,2\},\{3\},\emptyset)$
Figure 2: The 2-way elliptope $\mathcal{L}_{3,2}$ has 4 vertices (red points), corresponding to partitions of 3 distinguished elements into at most 2 sets.

Figure 3: The 3-way elliptope $\mathcal{L}_{3,3}$ has 5 vertices (red points), corresponding to partitions of 3 distinguished elements into at most 3 sets.
\( P_3 = (\{1, 3\}, \{2\}, \emptyset) \)
\( P_4 = (\{2, 3\}, \{1\}, \emptyset) \)
\( P_5 = (\{1\}, \{2\}, \{3\}) \)

Note that \( L_{n,k} \) is simply the elliptope intersected with an orthant. This characterization is useful to understand the geometric and combinatorial structure of \( L_{n,k} \). The difference between \( L_{n,r} \) and \( L_{n,s} \) is the amount by which the intersecting orthant is translated.

If we translate the orthant continuously from 0 to \(-1/(n-1)\) the vertex that represents the grouping of all elements into a single set remains fixed. This vertex is the matrix of all 1’s. On the other hand, the vertex that represents the partition of all elements into different sets only appears when the orthant reaches \(-1/(n-1)\). This vertex is the \( n \)-partition matrix with 1’s on the diagonal and \(-1/(n-1)\) in the off diagonal entries.

Let \( \Delta \) be a convex subset of \( \mathbb{R}^n \). For a point \( x \in \Delta \), the normal cone of \( \Delta \) at \( x \) is the set

\[
N(\Delta, x) = \{ y \in \mathbb{R}^n \mid y \cdot x \geq y \cdot z \ \forall z \in \Delta \}.
\]

A vertex of \( \Delta \) is (by definition) a point with a full-dimensional normal cone.

The following result shows that the normal cone of \( L_{n,k} \) at a \( k \)-partition matrix is full-dimensional.

**Proposition 4.** If \( X \in Q_{n,k} \) and \( \|Y - X\| < 1/(k-1) \) then \( Y \in N(L_{n,k}, X) \).

**Proof.** If \( \|Y - X\| < 1/(k-1) \) then \( \|Y - X\|_{i,j} < 1/(k-1) \) for all \( \{i,j\} \subseteq [n] \). Since \( X_{i,j} \) is either 1 or \(-1/(k-1) \) we can see that \( Y \) has the same sign pattern as \( X \). If \( Z \in L_{n,k} \) all of the entries in \( Z \) are between \(-1/(k-1) \) and 1. Therefore \( Y \cdot X \geq Y \cdot Z \).

The next proposition shows that \( k \)-partition matrices are the only matrices in \( L_{n,k} \) where every entry is either \(-1/(k-1) \) or 1.

**Proposition 5.** If \( X \in L_{n,k} \) and \( X_{i,j} \in \{-1/(k-1), 1\} \) for all \( \{i,j\} \subseteq [n] \) then \( X \in Q_{n,k} \).

**Proof.** Suppose \( X_{i,j} \in \{-1/(k-1), 1\} \) for all \( \{i,j\} \subseteq [n] \). Since \( X \) is a Gram matrix we know that \( X_{i,j} = 1 \) defines an equivalence relation on \([n]\). Let \((A_1, \ldots, A_l)\) be the equivalence classes of this relationship. If \( i \in A_r \) and \( j \in A_s \) with \( r \neq s \) then \( X_{i,j} = -1/(k-1) \). This means we have \( l \) unit vectors with the dot product between each pair equal to \(-1/(k-1) \). Lemma 4 in [5] implies that \( l \leq k \). We conclude \( X \in Q_{n,k} \).

Let

\[
T(M) = \arg \max_{X \in L_n} M \cdot X.
\]

We will use the following lemma from [8].

**Lemma 6.** Let \( M \in S(n) \) and \( X = T(M) \).

Suppose \( X \) is the Gram matrix of \( n \) unit vectors \((v_1, \ldots, v_n)\). Then,

(a) There exists real values \( \alpha_i \) such that

\[
\sum_{j \neq i} M_{i,j} v_j = \alpha_i v_i.
\]

(b) The vectors \((v_1, \ldots, v_n)\) are linearly dependent and \( \text{rank}(X) < n \).
(c) There exists a diagonal matrix $D$ such that,

$$MX = DX.$$ 

Now we are ready to prove the main result of this section, showing that the vertices of $\mathcal{L}_{n,k}$ are in fact the integer solutions to the Max $k$-Cut problem.

**Theorem 7.** The vertices of $\mathcal{L}_{n,k}$ are the $k$-partition matrices.

**Proof.** Suppose $X \in \mathcal{Q}_{n,k}$. Proposition A implies $N(\mathcal{L}_{n,k}, X)$ is full-dimensional.

Now suppose $X \notin \mathcal{Q}_{n,k}$. Proposition B implies $X$ must have an entry $X_{i,j} \notin \{-1/(k-1), 1\}$

Since $\mathcal{L}_{n,k} \subseteq \mathcal{L}_n$ we know $X \in \mathcal{L}_n$. Note that $X_{i,j} \notin \{-1, 1\}$. Let $J$ be a matrix with $J_{i,j} = J_{j,i} = 1$ and $J_{k,l} = 0$ for $\{k, l\} \neq \{i, j\}$.

Let $\mathcal{O}_{n,k} = \{X \mid X_{i,j} \geq -1/(k-1)\}$ be the orthant such that $\mathcal{L}_{n,k} = \mathcal{L}_n \cap \mathcal{O}_{n,k}$. We consider $N(\mathcal{L}_n, X)$ and $N(\mathcal{O}_{n,k}, X)$ separately and show both cones are orthogonal to $J$.

Suppose $M \in N(\mathcal{L}_n, X)$. Consider $A = M + \epsilon J$. We show $A \notin N(\mathcal{L}_n, X)$ for any $\epsilon \neq 0$. For the sake of contradiction suppose $A$ is in the normal cone of $X$. Then $X = T(M)$ and $X = T(A)$.

Since $X = T(A)$ by the lemma above we know $X$ is the Gram matrix of $(v_1, \ldots, v_n)$ where,

$$v_i \propto \sum_{k \neq i} M_{i,k}v_k.$$ 

and since $X = T(A)$ the lemma also implies,

$$v_i \propto \sum_{k \neq i} (M_{i,k} + \epsilon J_{i,k})v_k \Rightarrow v_i \propto \epsilon v_j + \sum_{k \neq i} M_{i,k}v_k.$$ 

Therefore

$$v_i \propto v_j.$$ 

Since $X_{i,j} \notin \{-1, 1\}$ the unit vectors $v_i$ and $v_j$ can not be proportional and we have a contradiction. Therefore $A$ cannot be in $N(\mathcal{L}_n, X)$. This implies $\epsilon J \notin N(\mathcal{L}_n, X)$ for any $\epsilon \neq 0$ and $N(\mathcal{L}_n, X)$ is orthogonal to $J$.

Now note

$$N(\mathcal{O}_{n,k}, X) = \text{cone}(\{e^{r,s} \mid X_{r,s} = -1/(k-1)\}),$$

where $e^{r,s}$ is the matrix that is 0 everywhere except in the $(r, s)$ position which has value 1. The product $J \cdot e^{r,s}$ equals 0 for all $(r, s)$ with $X_{r,s} = -1/(k-1)$. Therefore $N(\mathcal{O}_{n,k}, X)$ is orthogonal to $J$.

We conclude $N(\mathcal{L}_{n,k}, X) = \text{cone}(\{v \mid v \in N(\mathcal{L}_n, X) \cup N(\mathcal{O}_{n,k}, X)\})$ is orthogonal to $J$ and is not full-dimensional. \hfill \square

## 5 Iterated linear optimization and rounding

Let $\Delta \subset \mathbb{R}^n$ be a compact convex subset containing the origin. Let $T(x)$ be the map defined by linear optimization over $\Delta$,

$$T(x) = \text{argmax}_{y \in \Delta} x \cdot y.$$ 

In [8] it was shown that fixed point iteration with $T$ always converges to a fixed point. Furthermore, when $\Delta$ is the elliptope, $T(X)$ solves a relaxation to the closest vertex problem. Here we derive a similar result for the $k$-way elliptope, and show that iterated linear optimization in $\mathcal{L}_{n,k}$ can be used to round a solution to the SDP relaxation for Max $k$-Cut.
5.1 Deterministic rounding in $\mathcal{L}_{n,k}$

Let $X \in \mathcal{L}_{n,k}$ be a solution to the SDP relaxation of the Max $k$-Cut problem. If $X \in \mathcal{Q}_{n,k}$ then $X$ defines $k$-partition that is an optimal solution to the Max $k$-Cut problem. Otherwise we consider the problem of rounding $X$ by finding $Y \in \mathcal{Q}_{n,k}$ that is closest to $X$. By relaxing the problem we obtain a new SDP. Solving the new SDP leads to a new solution $Y \in \mathcal{L}_{n,k}$. If $Y \in \mathcal{Q}_{n,k}$ then it is the closest $k$-partition matrix to $X$. Otherwise we recursively look for a matrix $Z \in \mathcal{Q}_{n,k}$ that is closest to $Y$. The approach leads to a fixed point iteration process with a map $T'$ that optimizes a linear function over $\mathcal{L}_{n,k}$.

Let $A$ be the matrix where every entry is $(1-k)/2k$. If $Z \in \mathcal{Q}_{n,k}$ then all entries in $Z + A$ are in $\{- (k + 1)/2k, (k + 1)/2k\}$ and $(Z + A) \cdot (Z + A)$ is constant.

Consider the following expansion,

$$
||X - Y||^2 = ||(X + A) - (Y + A)||^2 = (X + A) \cdot (X + A) + (Y + A) \cdot (Y + A) - 2(X + A) \cdot (Y + A).
$$

Note that $(X + A) \cdot (X + A)$ does not depend on $Y$ and $(Y + A) \cdot (Y + A)$ is constant. Therefore the closest $k$-partition matrix to $X$ is,

$$
Y = \arg\min_{Y \in \mathcal{Q}_{n,k}} ||X - Y||^2 = \arg\max_{Y \in \mathcal{Q}_{n,k}} (X + A) \cdot (Y + A),
$$

$$
= \arg\max_{Y \in \mathcal{Q}_{n,k}} (X + A) \cdot Y.
$$

Relaxing this problem to $\mathcal{L}_{n,k}$ we obtain $Y = T(X + A)$ where $T$ is defined over $\Delta = \mathcal{L}_{n,k}$.

Let $T'(X) = T(X + A)$. That is,

$$
T'(X) = \arg\max_{Y \in \mathcal{L}_{n,k}} (X + A) \cdot Y.
$$

**Fixed point iteration** Our rounding method involves fixed point iteration with $T'$. That is, we generate a sequence $\{X_t\}$ where $X_0 = X$ and,

$$
X_{t+1} = T'(X_t).
$$

We say that a fixed point $x$ of a map $f : \Delta \to \Delta$ is *attractive* if $\exists \epsilon > 0$ such that $||x - x_0|| < \epsilon$ implies that iteration with $f$ starting at $x_0$ converges to $x$.

**Proposition 8.** The $k$-partition matrices are attractive fixed points of $T'$.

**Proof.** Let $X \in \mathcal{Q}_{n,k}$. Similar to Proposition 4 we can show that if $||Y - X|| < (k + 1)/2k$ then $T'(Y) = X$. This implies $X$ is an attractive fixed point of $T'$.

As discussed above, each step of the fixed point iteration process is solving a relaxation to the closest $k$-partition matrix problem. Moreover, $k$-partition matrices are fixed points of $T'$. So if $X_t$ is a $k$-partition matrix, then the sequence converges to $X_t$.

Figure 4 shows the result of the fixed point iteration process in $\mathcal{L}_{n,k}$ for different values of $k$. In each case we start from the result of the SDP relaxation of Max $k$-Cut for a graph with $n = 50$ vertices and random weights. In each example fixed point iteration with $T'$ converges to a
Figure 4: Fixed point iteration with $T'$, starting from the solution of the SDP relaxation of Max $k$-Cut for a graph with 50 vertices and random weights. To visualize a matrix in $L_{n,k}$ we show an $n \times n$ picture with a pixel for each entry in the matrix. Bright yellow pixels indicate entries with high value, and dark blue pixels indicate entries with low value. In each case we obtain a sequence of solutions that converge to a $k$-partition matrix. The rows and columns in each example have been permuted so the final matrix is block diagonal to facilitate visualization.
k-partition matrix after a small number of iterations. Figure 1 in Section 1 shows an example of the sequence of solutions generated by $T'$ for a geometric clustering problem.

Iteration with $T'$ is equivalent to iteration with $T$ in $\Delta = L_{n,k} + A$. Thus, the convergence results from [8] imply the sequence $\{X_t\}$ converges to a fixed point of $T'$. We have shown that matrices in $Q_{n,k}$ are attractive fixed points of $T'$. Although the map $T'$ has other fixed points, our numerical experiments suggest that fixed point iteration with $T'$ starting from a generic point always converges to a $k$-partition matrix.

6 Experiments

In this section we illustrate experimental clustering results with geometric datasets. The algorithms were implemented in Python and run on a computer with an Intel i7 CPU @ 2.6 Ghz with 8GB of RAM. We use the cvxpy package for convex optimization together with the SCS (splitting conic solver) package to solve SDPs. The fixed point iteration process we use for rounding involves solving a sequence of SDPs identical to the Max $k$-Cut SDP but with a different objective. For the examples below solving each SDP took 2 to 3 minutes, and the fixed point iteration method converged after 1 to 3 iterations.

In each clustering experiment we have a dataset $D = \{x_1, \ldots, x_n\}$ with $x_i \in \mathbb{R}^2$. We use points in $\mathbb{R}^2$ to facilitate the visualization of the data but the approach can be directly applied for clustering points in $\mathbb{R}^d$. As discussed in Section 2 we cluster the data by defining a Max $k$-Cut problem with weights $M_{i,j} = ||x_i - x_j||^2$. With this choice of weights the maximum weight partition should lead to compact clusters where points in different clusters are far from each other and points within a single cluster are close to each other.

Figures 5, 6, and 7 illustrate the results of clustering a dataset of 200 points into 5, 10 and 20 clusters respectively. In each case we compare the result obtained using fixed point iteration for rounding the SDP relaxation to the result of randomized rounding. For the randomized rounding method we repeat the rounding procedure 50 times and select the partition with highest weight generated over all trials.

In all of the experiments we see that the weight of the partition generated by the fixed point iteration method is higher than the weight of the best partition generated by randomized rounding. When $k = 5$ (Figure 5) the results of the two methods are similar, but the weight of the partition generated by fixed point iteration is slightly better. When $k = 10$ and $k = 20$ (Figures 6 and 7) the results of randomized rounding are significantly degraded while the results of the fixed point iteration method remain very good.

Figure 8 illustrates the partitions obtained in different trials of randomized rounding for the case when $k = 5$. We can see there is a lot of variance in the results and that the random rounding method often leads to poor clusterings even when $k$ is relatively small. The result of our fixed point iteration method in the same data is shown in Figure 5(c).

Figure 9 shows an example where the input data has 160 points generated by sampling 20 points from 8 different Gaussian distributions. The Gaussian distributions have standard deviation $\sigma = 0.2$ and means arranged around a circle of radius 1. In this case there is a ground truth clustering where points are grouped according to the Gaussian used to generate them. The overlap between the distributions is sufficiently high that it is impossible to recover the ground truth clustering perfectly, but the result of the fixed point iteration method is closely aligned with the ground truth. The results of randomized rounding are not as good even when we select the best of
Figure 5: Clustering 200 pts with $k = 5$. 
Figure 6: Clustering 200 pts with $k = 10$. 

(a) Input data 

(b) Randomized (best of 50) $w(C) = 3587153$ 

(c) Fixed point $w(C) = 3701677$
Figure 7: Clustering 200 pts with $k = 20$. 

(a) Input data

(b) Randomized (best of 50) $w(C) = 3658976$

(c) Fixed point $w(C) = 3722073$
Figure 8: Clustering 200 pts with $k = 5$ and randomized rounding. The result of the fixed point iteration method in the same data is shown in Figure 5(c).
|               | $w(C)/w(D)$ | Rand index   |
|---------------|-------------|--------------|
| minimum       | 1.005       | fixed point  | 0.972 ± 0.006 |
| maximum       | 1.026       | randomized rounding | 0.935 ± 0.018 |
| mean          | 1.014       |              |               |

Table 1: Experiments with 10 different datasets generated by a mixture of Gaussians (see Figure 9).

(a) Partition weights

(b) Clustering accuracy

50 trials of the randomized procedure.

We repeated the last experiment 10 times to quantify the difference between the two rounding methods. Each repetition was done with a new dataset generated from the mixture of Gaussians. The fixed point iteration method always produced a partition with higher weight. Table 1(a) summarizes the minimum, maximum, and mean value of the ratio $w(C)/w(D)$, where $C$ is the partition produced by the fixed point iteration method and $D$ is the result of the best of 50 trials of randomized rounding. We also compare the resulting clusterings to the ground truth using the Rand index ([19]). The Rand index is a number between 0 and 1 measuring the agreement between two clusterings. Let $A$ and $B$ be clusterings. Let $a$ be the number of pairs of elements that are in the same cluster in both $A$ and $B$ while $b$ is the number of pairs of elements that are in different clusters in both $A$ and $B$. The Rand index is,

$$R(A, B) = \frac{a + b}{\binom{n}{2}}.$$  

We see in Table 1(b) that the fixed point rounding method consistently produces a clustering that is more similar to the ground truth than the randomized rounding method.

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Figure 9: Clustering 160 pts sampled from 8 Gaussians with $k = 8$. 

(a) Input data a ground truth clustering

(b) Randomized (best of 50) $w(C) = 26837$

(c) Fixed point $w(C) = 27158$
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