

The ratio-cut polytope and K-means clustering ^{*}

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Abstract

We introduce the ratio-cut polytope defined as the convex hull of ratio-cut vectors corresponding to all partitions of n points in \mathbb{R}^m into at most K clusters. This polytope is closely related to the convex hull of the feasible region of a number of clustering problems such as K-means clustering and spectral clustering. We study the facial structure of the ratio-cut polytope and derive several types of facet-defining inequalities. We then consider the problem of K-means clustering and introduce a novel linear programming (LP) relaxation for it. Subsequently, we focus on the case of two clusters and derive a sufficient condition under which the proposed LP relaxation recovers the underlying clusters exactly. Namely, we consider the stochastic ball model, a popular generative model for K-means clustering, and we show that if the separation distance between cluster centers satisfies $\Delta > 1 + \sqrt{3}$, then the LP relaxation recovers the planted clusters with high probability. This is a major improvement over the only existing recovery guarantee for an LP relaxation of K-means clustering stating that recovery is possible with high probability if and only if $\Delta > 4$. Our numerical experiments indicate that the proposed LP relaxation significantly outperforms a popular semidefinite programming relaxation in recovering the planted clusters.

Key words. *Ratio-cut polytope; K-means clustering; Linear programming, Stochastic ball model.*

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1 Introduction

Clustering is concerned with partitioning a given set of data points $\{x^i\}_{i=1}^n$ in \mathbb{R}^m into K subsets such that some dissimilarity function among the points is minimized. Consider a partition of $[n] := \{1, \dots, n\}$; i.e., $\{\Gamma_k\}_{k=1}^K$ such that $\Gamma_a \cap \Gamma_b = \emptyset$ for all $a, b \in [K] := \{1, \dots, K\}$ and $\cup_{k \in [K]} \Gamma_k = [n]$, where we further assume $\Gamma_k \neq \emptyset$ for all $k \in [K]$. *K-means*

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clustering partitions the data points into K clusters by minimizing the total squared distance between each data point and the corresponding cluster center:

$$\begin{aligned} \min \quad & \sum_{k=1}^K \sum_{i \in \Gamma_k} \left\| x^i - \frac{1}{|\Gamma_k|} \sum_{j \in \Gamma_k} x^j \right\|_2^2 \\ \text{s.t.} \quad & \{\Gamma_k\}_{k \in [K]} \text{ is a partition of } [n]. \end{aligned} \quad (1)$$

It is well-known that Problem (1) is NP-hard even when there are only two clusters [6] or when the data points are in \mathbb{R}^2 [20]. The most famous heuristic for K-means clustering is Lloyd’s algorithm [18] which, in spite of its effectiveness, in practice may converge to a local minimum that is arbitrarily bad compared to the global minimum [15]. Moreover, numerous constant-factor approximation algorithms have been developed, both for the fixed number of clusters K and for the fixed dimension m (see for example [15, 11]). In this paper, we are interested in the quality of convex relaxations for K-means clustering.

Several equivalent reformulations of K-means clustering, including a nonlinear binary program [26], a binary semidefinite program (SDP) [23], and a completely positive program [25] are given in the literature. In the following, we present an alternative formulation that we will use to construct our new convex relaxation (see [16] for the derivation). Consider partition of $[n]$; let $\mathbf{1}_{\Gamma_k}$, $k \in [K]$ be the indicator vector of the k th cluster; i.e., the i th component of $\mathbf{1}_{\Gamma_k}$ is defined as: $(\mathbf{1}_{\Gamma_k})_i = 1$ if $i \in \Gamma_k$ and $(\mathbf{1}_{\Gamma_k})_i = 0$ otherwise. Define the *partition matrix* as

$$Z = \sum_{k=1}^K \frac{1}{|\Gamma_k|} \mathbf{1}_{\Gamma_k} \mathbf{1}_{\Gamma_k}^T. \quad (2)$$

Denote by $D \in \mathbb{R}^{n \times n}$ the distance matrix with the (i, j) th entry given by $d_{ij} = \|x^i - x^j\|_2^2$. Then it can be shown that Problem (1) can be equivalently written as:

$$\begin{aligned} \min \quad & \sum_{i,j \in [n]} d_{ij} Z_{ij} \\ \text{s.t.} \quad & Z \text{ is a partition matrix defined by (2)}. \end{aligned} \quad (3)$$

SDP relaxations. The most popular convex relaxations for K-means clustering are SDP relaxations; indeed, both theoretical and numerical properties of these algorithms have been extensively investigated in the literature (see for example [24, 23, 25]). These relaxations are obtained by observing that any partition matrix Z satisfies the following properties:

$$\begin{aligned} Z \mathbf{1}_n &= \mathbf{1}_n, \quad \text{Tr}(Z) = K, \\ Z &\succeq 0, \quad Z \geq 0, \end{aligned} \quad (4)$$

where $\mathbf{1}_n$ is a n -vector with all entries equal to 1 and $\text{Tr}(Z)$ is the trace of the matrix Z . Moreover, $Z \succeq 0$ and $Z \geq 0$ mean that the matrix Z is positive semidefinite and component-wise nonnegative, respectively. A widely-studied SDP relaxation of the K-means clustering, often referred to as “Peng-Wei relaxation” [23], is given by

$$\begin{aligned} \min \quad & \sum_{i,j \in [n]} d_{ij} Z_{ij} \\ \text{s.t.} \quad & Z \mathbf{1}_n = \mathbf{1}_n, \quad \text{Tr}(Z) = K, \quad Z \succeq 0, \quad Z \geq 0, \quad Z = Z^T. \end{aligned} \quad (5)$$

If by solving Problem (5), we obtain a minimizer \bar{Z} that is a partition matrix as defined by (2), then \bar{Z} is also optimal for the original problem, as the feasible region of Problem (5) contains the feasible region of Problem (3). Otherwise, a common approach is to devise a *rounding scheme* to extract a feasible solution of (3) from the relaxation solution \bar{Z} . This two-phase approach has been successfully employed for clustering various synthetic and real data sets [23, 25].

Recovery guarantees under stochastic models. A recent stream of research in data clustering is concerned with obtaining conditions under which a planted clustering corresponds to the unique optimal solution of a SDP relaxation under suitable generative models [4, 2, 12, 22, 14, 5, 3, 17, 16]. Such conditions are often referred to as *exact recovery* (henceforth, simply *recovery*) conditions. Generally speaking, these works first provide deterministic sufficient conditions for a given clustering assignment to be the unique optimal solution of a SDP relaxation via the construction of dual certificates. Subsequently, they show that those conditions hold with high probability under a given random model. Throughout this paper, we say that an optimization problem *recovers* the planted clusters if its unique optimal solution corresponds to the planted clusters.

The stochastic ball model (SBM) is the most widely-studied generative model for K-means clustering. In this distributional setting, we assume that there exist K clusters in \mathbb{R}^m and the data in each cluster consists of $\frac{n}{K}$ points sampled from a uniform distribution within a ball of unit radius. The question is what is the *minimum separation distance* Δ between cluster centers needed for a convex relaxation to recover these K clusters with high probability (i.e., probability tending to 1 as $n \rightarrow \infty$). Clearly, a convex relaxation recovers the planted clusters only if the original K-means problem succeeds in doing so. Perhaps surprisingly, the recovery threshold for K-means clustering under the SBM remains an open question. Recently, in [6], the authors prove that when the points are generated uniformly on two m -dimensional touching spheres for $m \geq 3$, in the limit, i.e., when the empirical samples is replaced by the probability measure, K-means clustering identifies the two individual spheres as the two clusters. In this paper, we show that the same recovery result is valid for the SBM.

In [4], the authors consider the Peng-Wei relaxation as defined by (5) and show that if $\Delta > 2\sqrt{2}(1 + 1/\sqrt{m})$, then the SDP recovers the planted clusters with high probability. In [14], the authors consider the same SDP and prove that recovery is guaranteed with high probability if $\Delta > 2 + K^2/m$, which is near optimal in $m \gg K^2$ regime. The authors of [16] obtain yet another recovery condition for Peng-Wei relaxation given by $\Delta > 2 + O(\sqrt{K/m})$ which is an improvement over the previous condition when K is large. Moreover, in [16], the authors prove that if $\Delta < 1 + \sqrt{1 + 2/(m + 2)}$, then with high probability, Peng-Wei relaxation fails in recovering the planted clusters.

LP relaxations. It is widely accepted that state-of-the-art LP solvers outperform the SDP counterparts in both speed and scalability. However, for K-means clustering, to date, there exists no LP relaxation with desirable theoretical or computational properties. In [4], the authors consider the following LP relaxation of K-means clustering:

$$\begin{aligned} \min \quad & \sum_{i,j \in [n]} d_{ij} Z_{ij} \\ \text{s.t.} \quad & Z\mathbf{1}_n = \mathbf{1}_n, \quad \text{Tr}(Z) = K, \quad Z \geq 0, \quad Z = Z^T, \quad Z_{ij} \leq Z_{ii}, \quad \forall i, j \in [n]. \end{aligned} \tag{6}$$

Subsequently, they show that under the SBM, Problem (6) recovers the planted clusters with high probability if and only if $\Delta > 4$. We should remark that if $\Delta > 4$, any two points within a particular cluster are closer to each other than any two points from different clusters, and hence in this case, recovery follows from a simple distance thresholding. They complement this negative theoretical result with poor numerical performance to conclude the ineffectiveness of the “natural” LP relaxation for K-means clustering. In [8, 9], the authors study the recovery properties of LP relaxations for community detection and joint object matching.

Our contribution. In this paper, we propose a novel LP relaxation for K-means clustering with favorable theoretical and numerical properties. We start by introducing the *ratio-cut polytope* RCut_n^K defined as the convex hull of ratio-cut vectors corresponding to all assignments of n points to at most K nonempty clusters. We are interested in a certain facet of RCut_n^K , denoted by $\text{RCut}_n^{=K}$, which corresponds to all ratio-cut vectors of exactly K nonempty clusters. As we detail later, $\text{RCut}_n^{=K}$ is the polytope obtained by projecting out variables Z_{ii} , $i \in [n]$ from convex hull of the feasible region of Problem (3). We then study the facial structures of RCut_n^K and $\text{RCut}_n^{=K}$ and derive several classes of facet-defining inequalities for these polytopes. This in turn enables us to obtain a new LP relaxation for K-means clustering. We then address the question of recovery when there are two clusters. First, we obtain a deterministic sufficient condition under which the planted clusters correspond to an optimal solution of the LP relaxation. Subsequently, we focus on the SBM, and prove that if $\Delta > 1 + \sqrt{3}$, the LP relaxation recovers the planted clusters with high probability. While this recovery guarantee is significantly better than the recovery guarantee of Problem (6), our empirical observations suggest that it is overly conservative. Indeed, our numerical experiments on a collection of randomly generated test problems indicate that the LP relaxation outperforms the Peng-Wei SDP relaxation.

Organization. The remainder of the paper is structured as follows. In Section 2, we study the facial structure of the ratio-cut polytope. In Section 3 we introduce a new LP relaxation for K-means clustering. We then focus on the case of two clusters and obtain a deterministic sufficient condition under which the planted clusters correspond to an optimal solution of the LP relaxation. In Section 4, we consider the K-means clustering problem with two clusters under the SBM. We first show that for dimension $m \geq 3$, in the continuum limit, the K-means clustering problem achieves optimal recovery threshold. Next, utilizing our deterministic condition of Section 3, we obtain a recovery guarantee for the LP relaxation. We present our numerical experiments in Section 5. Finally, proofs of the technical results omitted in Section 4 are given in Section 6.

2 The ratio-cut polytope

In this section, we perform a polyhedral study of the convex hull of the feasible region of Problem (3). Denote by $\{x^i\}_{i=1}^n$ a set of points in \mathbb{R}^m that we would like to put into at most K clusters. Consider a partition of $[n]$ denoted by $\{\Gamma_k\}_{k=1}^K$ where some of the partitions Γ_k could be empty. For any $1 \leq i < j \leq n$, define $X_{ij} = \frac{1}{|\Gamma_k|}$ if i and j belong to the same partition Γ_k , for some $k \in [K]$ and $X_{ij} = 0$ if i and j are in different partitions. Let X be the $\binom{n}{2}$ -vector whose elements are X_{ij} . We refer to any such vector X as a *ratio-cut vector* and we refer to the convex hull in $\mathbb{R}^{\binom{n}{2}}$ of all ratio-cut vectors

corresponding to *at most* K nonempty clusters as the *ratio-cut polytope* and denote it by RCut_n^K . Throughout the paper, we let $X_{ji} = X_{ij}$ whenever $i < j$. If $K = 1$, then RCut_n^K is given by $\text{RCut}_n^1 = \{X : X_{ij} = \frac{1}{n}, \forall 1 \leq i < j \leq n\}$. Moreover, it can be shown that $\text{RCut}_n^2 = \{X_{12} : 0 \leq X_{12} \leq 1/2\}$. Henceforth, we assume that $n \geq 3$ and $2 \leq K \leq n$.

We denote by $\text{RCut}_n^{\neq K}$ the convex hull of all ratio-cut vectors corresponding to *exactly* K nonempty clusters. If $K = n$, it follows that $\text{RCut}_n^{\neq n} = \{X : X_{ij} = 0, \forall 1 \leq i < j \leq n\}$ and if $K = n - 1$, it can be shown that

$$\text{RCut}_n^{\neq n-1} = \left\{ X : \sum_{1 \leq i < j \leq n} X_{ij} = \frac{1}{2}, X_{ij} \geq 0, \forall 1 \leq i < j \leq n \right\}.$$

Henceforth, when studying the facial structure of $\text{RCut}_n^{\neq K}$, we assume that $n \geq 4$ and $2 \leq K \leq n - 2$. See Figure 1 for an illustration of RCut_n^K and $\text{RCut}_n^{\neq K}$, with $n = 3$ and $K = 2$.

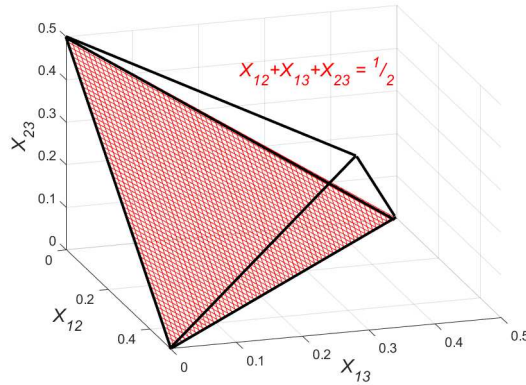


Figure 1: The polytopes RCut_n^K and $\text{RCut}_n^{\neq K}$, with $n = 3$ and $K = 2$. The ratio-cut polytope RCut_n^K is the convex hull of the ratio-cut vectors $\{(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}), (\frac{1}{2}, 0, 0), (0, \frac{1}{2}, 0), (0, 0, \frac{1}{2})\}$. The polytope $\text{RCut}_n^{\neq K}$, shaded in red, is a facet of RCut_n^K whose affine hull is given by $X_{12} + X_{13} + X_{23} = \frac{1}{2}$.

Consider the convex hull of the feasible region of Problem (3) denoted by \mathcal{Z}_n^K ; i.e., the convex hull of all partition matrices Z . It then follows that

$$\text{RCut}_n^{\neq K} = \left\{ X \in \mathbb{R}^{\binom{n}{2}} \mid \exists Z \in \mathcal{Z}_n^K : X_{ij} = Z_{ij}, \forall 1 \leq i < j \leq n \right\}. \quad (7)$$

That is, the polytope $\text{RCut}_n^{\neq K}$ is obtained by projecting out diagonal variables $Z_{ii}, i \in [n]$ from the convex hull of partition matrices. Hence, understanding the facial structure of $\text{RCut}_n^{\neq K}$ enables us to construct a strong LP relaxation for K-means clustering. By definition, $\text{RCut}_n^K \supset \text{RCut}_n^{\neq K}$. However, we are interested in studying RCut_n^K due to its following fundamental property.

Proposition 1. *The ratio-cut polytope RCut_n^K with $n \geq 3$ and $2 \leq K \leq n$ is full-dimensional; i.e., $\dim(\text{RCut}_n^K) = \binom{n}{2}$.*

Proof. Since $\text{RCut}_n^K \subset \text{RCut}_n^{K'}$ for all $K' > K$, to prove the statement, it suffices to show that RCut_n^K contains $\binom{n}{2} + 1$ affinely independent points.

First let $n \neq 4$. Consider the ratio-cut vector corresponding to one cluster; i.e., $X_{ij} = \frac{1}{n}$ for all $1 \leq i < j \leq n$ and the $\binom{n}{2}$ ratio-cut vectors corresponding to two clusters

of cardinality two and $n - 2$; i.e., for any $1 \leq r < s \leq n$, consider the ratio-cut vector with $X_{rs} = \frac{1}{2}$, $X_{ij} = \frac{1}{n-2}$ if $i \notin \{r, s\}$ and $j \notin \{r, s\}$, and $X_{ij} = 0$, otherwise. It can be checked that these $\binom{n}{2} + 1$ ratio-cut vectors are affinely independent.

Now consider $n = 4$; in this case RCut_4^2 is the convex hull of eight ratio-cut vectors and it can be checked that any seven of these vectors containing the ratio-cut vector corresponding to one cluster are affinely independent. Notice that we could not utilize the same construction as the one we used for $n \neq 4$ since due to symmetry, for $n = 4$, the set of all ratio-cut vectors corresponding to two clusters of cardinality two and $n - 2$ consists of $\frac{1}{2}\binom{n}{2} = 3$ affinely independent points. \square

2.1 Three types of facets of RCut_n^K and $\text{RCut}_n^{=K}$

In the next three propositions, we present various classes of facet-defining inequalities for RCut_n^K and $\text{RCut}_n^{=K}$. These results enable us to construct a strong LP relaxation for K-means clustering.

Proposition 2. *The inequality*

$$\sum_{1 \leq i < j \leq n} X_{ij} \geq \frac{n - K}{2} \quad (8)$$

is valid for RCut_n^K and is facet-defining if and only if $K \leq n - 1$. Moreover, the affine hull of $\text{RCut}_n^{=K}$ is defined by the equation

$$\sum_{1 \leq i < j \leq n} X_{ij} = \frac{n - K}{2}. \quad (9)$$

Proof. Consider a partition of $[n]$ given by $\{\Gamma_k\}_{k=1}^K$; denote by \mathcal{K}_1 the subset of $[K]$ for which $|\Gamma_k| = 1$ and denote by \mathcal{K}_2 the subset of $[K]$ for which $|\Gamma_k| \geq 2$. It then follows that

$$\sum_{1 \leq i < j \leq n} X_{ij} = \sum_{k \in \mathcal{K}_2} \frac{1}{|\Gamma_k|} \binom{|\Gamma_k|}{2} = \frac{1}{2} \left(\sum_{k \in \mathcal{K}_2} |\Gamma_k| - |\mathcal{K}_2| \right) = \frac{n - |\mathcal{K}_1| - |\mathcal{K}_2|}{2} \geq \frac{n - K}{2},$$

where the last inequality holds with equality when $K = |\mathcal{K}_1| + |\mathcal{K}_2|$; i.e., when all Γ_k , $k \in [K]$ are nonempty; that is, we have exactly K clusters.

Now let $K \leq n - 1$ and consider a facet-defining inequality $aX \geq \alpha$ for RCut_n^K that is satisfied tightly by all ratio-cut vectors that are binding for inequality (8). We show that the two inequalities coincide up to a positive scaling which by full dimensionality of the ratio-cut polytope (see Proposition 1), implies that inequality (8) defines a facet of RCut_n^K .

Consider a partition of $[n]$ with K nonempty clusters Γ_k , $k \in [K]$ with $\Gamma_1 = \{i\}$ for some $i \in [n]$. Consider a second partition obtained by switching point i with a point j where $j \in \Gamma_r$ for some $|\Gamma_r| \geq 2$. Note such a Γ_r always exists since by assumption $K \leq n - 1$. Substituting the corresponding ratio-cut vectors in $aX = \alpha$ and subtracting the resulting equalities, we obtain:

$$\sum_{l \in \Gamma_r \setminus \{i, j\}} a_{jl} = \sum_{l \in \Gamma_r \setminus \{i, j\}} a_{il}. \quad (10)$$

Next, take the two partitions defined above and for each one, remove a point $k \neq i, j$ from Γ_r and place it in Γ_1 . Substituting the corresponding ratio-cut vectors in $aX = \alpha$ yields:

$$\frac{a_{ik}}{2} + \frac{\sum_{l \in \Gamma_r \setminus \{i,j,k\}} a_{jl}}{|\Gamma_r| - 1} = \frac{a_{jk}}{2} + \frac{\sum_{l \in \Gamma_r \setminus \{i,j,k\}} a_{il}}{|\Gamma_r| - 1}. \quad (11)$$

From (10) and (11) it follows that $a_{ik} = a_{jk}$ for all distinct $i, j, k \in [n]$. Moreover it can be checked that for any ratio-cut vector associated to K nonempty clusters we have $\sum_{1 \leq i < j \leq n} X_{ij} = (n-K)/2$. Hence, if $K \leq n-1$, the inequality $aX \geq \alpha$ coincides with (8) up to a positive scaling implying that inequality (8) is facet-defining.

Now let $n = K$; in this case, the right-hand side of inequality (8) is zero and hence is implied by valid inequalities $X_{ij} \geq 0$ for all $1 \leq i < j \leq n$. Therefore, in this case inequality (8) is not facet-defining.

Finally, since the set of all ratio-cut vectors corresponding to K nonempty clusters constitute the set of tight points of the facet-defining inequality (8), we conclude that $\dim(\text{RCut}_n^{=K}) = \binom{n}{2} - 1$ for all $K \leq n-1$ and its affine hull is induced by $\sum_{1 \leq i < j \leq n} X_{ij} = (n-K)/2$. \square

Next, we present a class of facet-defining inequalities for the ratio-cut polytope that can be considered as the generalization of the well-known triangle inequalities associated with the cut polytope [10] (see Subsection 2.2 for more detail).

Proposition 3. *Let $l \in [n]$ and let T be a nonempty subset of $[n] \setminus \{l\}$. Then the inequality*

$$2 \sum_{j \in T} X_{lj} + \sum_{j \in [n] \setminus T \cup \{l\}} X_{lj} \leq 1 + \sum_{i,j \in T: i < j} X_{ij}, \quad (12)$$

is valid for RCut_n^K . Moreover, if $2 \leq |T| \leq K$, then inequality (12) defines a facet of RCut_n^K , and if in addition, $K \leq n-2$ then this inequality defines a facet of $\text{RCut}_n^{=K}$.

Proof. Denote by ω the number of points in T that are in the same cluster as l and let Ω denote the size of the corresponding cluster; clearly $\omega \geq 0$ and $\Omega \geq 1$. Then $\sum_{j \in T} X_{lj} = \frac{\omega}{\Omega}$ and $\sum_{j \in [n] \setminus T \cup \{l\}} X_{lj} = \frac{\Omega - \omega - 1}{\Omega}$. Moreover, if $\omega \geq 2$, we have $\sum_{i,j \in T} X_{ij} \geq \binom{\omega}{2} \frac{1}{\Omega}$. Hence to show the validity of inequality (12) it suffices to show that $1 + \frac{\omega-1}{\Omega} \leq 1$, if $\omega \in \{0, 1\}$ and $1 + \frac{\omega-1}{\Omega} \leq 1 + \frac{\omega(\omega-1)}{2\Omega}$, if $\omega \geq 2$, both of which are valid.

Let $K \in \{2, \dots, n\}$; we now show that if $t := |T| \in \{2, \dots, \min\{n-1, K\}\}$, then inequality (12) defines a facet of RCut_n^K . Denote by

$$aX \leq \alpha, \quad (13)$$

a nontrivial valid inequality for RCut_n^K that is satisfied tightly by all ratio-cut vectors that are binding for (12). We show that inequalities (12) and (13) coincide up to a positive scaling, which by full dimensionality of RCut_n^K (see Proposition 1) implies that (12) defines a facet of RCut_n^K .

Let Γ_k , $k \in [K]$ form a partition of $[n]$. Assume that (i) $l \in \Gamma_1$, (ii) $|\Gamma_1 \cap T| = 1$ or $|\Gamma_1 \cap T| = 2$ and (iii) $|\Gamma_k \cap T| \leq 1$ for all $k \in [K] \setminus \{1\}$. It can be checked that the ratio-cut vector corresponding to any partition satisfying conditions (i)-(iii) satisfies (12) tightly. Note that all such partitions consist of at least t nonempty clusters if $|\Gamma_1 \cap T| = 1$ and at least $t-1$ nonempty clusters if $|\Gamma_1 \cap T| = 2$, all of which correspond to valid ratio-cut vectors in RCut_n^K since by assumption $2 \leq t \leq K$. Henceforth, by a ‘‘binding

partition,” we imply a partition of $[n]$ consisting of at most K nonempty clusters, which satisfies conditions (i)-(iii) above. In the following we present several types of binding partitions and by substituting the corresponding ratio-cut vectors in $aX = \alpha$, we prove the facetness of inequality (12).

Take some $r \in T$ and some $s \in [n] \setminus (T \cup \{l\})$. Consider a binding partition consisting of $q \leq K - 1$ nonempty clusters such that $\Gamma_2 = \{r, s\}$. Note that this binding partition exists since by assumption $t \geq 2$. Moreover, such a partition with exactly $K - 1$ nonempty clusters exists if $K \leq n - 1$. Now consider another binding partition consisting of $q + 1$ nonempty clusters, obtained from the above partition by removing s from Γ_2 and putting it in Γ_{q+1} . Substituting the ratio-cut vectors in $aX = \alpha$ we obtain $a_{rs} = 0$.

For any $j \in [n] \setminus (T \cup \{l, s\})$, consider a binding partition such that $\Gamma_2 = \{r, s\}$ and $\Gamma_3 = \{j\}$. Such a partition with exactly K nonempty clusters exists if $K \leq n - 2$. Construct a second binding partition from the above partition by swapping j and s . Substituting the ratio-cut vectors in $aX = \alpha$ and using $a_{rs} = 0$, we obtain $a_{rj} = 0$ for all $j \in [n] \setminus (T \cup \{l\})$. Similarly, we obtain $a_{sj} = 0$ for all $j \in [n] \setminus (T \cup \{l, s\})$.

For any $i \in T$ and for any $j \in [n] \setminus (T \cup \{l\})$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 2$) such that $\Gamma_2 = \{r, j\}$ and $\Gamma_3 = \{i\}$. Construct a second binding partition from the above partition by swapping r and i . Substituting the ratio-cut vectors in $aX = \alpha$ and using $a_{rj} = 0$, we obtain

$$a_{ij} = 0, \quad \forall i \in T, j \in [n] \setminus (T \cup \{l\}). \quad (14)$$

For any $i, j \in [n] \setminus (T \cup \{l\})$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 2$) such that $\Gamma_2 = \{s, j\}$ and $\Gamma_3 = \{i\}$. Construct a second binding partition from the above partition by swapping s and i . Substituting the ratio-cut vectors in $aX = \alpha$ and using $a_{sj} = 0$, we obtain

$$a_{ij} = 0, \quad \forall i, j \in [n] \setminus (T \cup \{l\}). \quad (15)$$

For any $i, j \in T$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 1$) with $\Gamma_1 = \{1, i\}$ and $\Gamma_2 = \{j\}$. Construct a second binding partition from the above partition by swapping i and j . Substituting the ratio-cut vectors in $aX = \alpha$, we obtain

$$a_{li} = \beta, \quad \forall i \in T. \quad (16)$$

For any $i, j \in [n] \setminus (T \cup \{l\})$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 1$) with $|\Gamma_1 \cap T| = 1$, $i \in \Gamma_1$, and $j \in \Gamma_2$. Construct a second binding partition from the above partition by swapping i and j . Substituting the ratio-cut vectors in $aX = \alpha$ and using (14)-(16), we obtain

$$a_{li} = \gamma, \quad \forall i \in [n] \setminus (T \cup \{l\}). \quad (17)$$

For any $i, j, k \in T$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 2$) with $\Gamma_1 = \{l, i, j\}$ and $\Gamma_2 = \{k\}$. Construct a second binding partition from the above partition by swapping j and k . Substituting the ratio-cut vectors in $aX = \alpha$ and using (16), we obtain

$$a_{ij} = \zeta, \quad \forall i, j \in T. \quad (18)$$

For any $i, j \in T$ and $k \in [n] \setminus (T \cup \{l\})$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 2$) with $\Gamma_1 = \{l, i, j\}$ and $\Gamma_2 = \{k\}$. Construct a

second binding partition from the above partition by swapping j and k . Substituting the ratio-cut vectors in $aX = \alpha$ and using (14)- (18), we obtain

$$\beta + \zeta = \gamma. \quad (19)$$

For any $i, j \in T$ and $k \in [n] \setminus (T \cup \{l\})$, consider a binding partition (consisting of K nonempty clusters, if $K \leq n - 2$) with $\Gamma_1 = \{l, i\}$ and $\Gamma_2 = \{j, k\}$. Construct a second binding partition from the above partition by adding j to Γ_1 . Substituting the ratio-cut vectors in $aX = \alpha$ and using (14), (16), and (18), we obtain

$$\beta + 2\zeta = 0. \quad (20)$$

Consider a binding partition, consisting of K nonempty clusters if $K \leq n - 1$, with $\Gamma_1 = \{l, i\}$ for some $i \in T$. Substituting the corresponding ratio cut vector in $aX = \alpha$ and using (14)-(16) yields $\beta = 2\alpha$. Together with (19) and (20), this in turn implies that inequality (13) can be equivalently written as $\alpha(2 \sum_{j \in T} X_{lj} + \sum_{j \notin T \cup \{l\}} X_{1j} - \sum_{i, j \in T, i < j} X_{ij}) \leq \alpha$ where $\alpha > 0$ since by assumption, inequality (13) is nontrivial and inequality (12) is valid, and this concludes the proof of facetness for RCut_n^K .

Finally, let us consider the polytope $\text{RCut}_n^{=K}$ for $2 \leq K \leq n - 2$. In the above proof, with the exception of the first one, all of the binding partitions consist of K nonempty clusters and hence the corresponding ratio-cut vectors are present in $\text{RCut}_n^{=K}$. As $\text{RCut}_n^{=K}$ is a facet of RCut_n^K , it follows that the inequality (12) defines a facet of $\text{RCut}_n^{=K}$. \square

Now consider the valid inequalities $X_{ij} \geq 0$ for all $1 \leq i < j \leq n$. As we show in the following, if $K \geq 3$, these inequalities define facets of the ratio-cut polytope.

Proposition 4. *Let $K \leq n - 1$. Then inequalities $X_{ij} \geq 0$ for all $1 \leq i < j \leq n$ define facets of RCut_n^K and $\text{RCut}_n^{=K}$ if and only if $K \geq 3$.*

Proof. We show without loss of generality that $X_{12} \geq 0$ defines a facet of RCut_n^K if and only if $K \geq 3$. First suppose that $K \geq 3$. It then follows that $X_{12} \geq 0$ is binding at all ratio-cut vectors in which 1 and 2 are not in the same cluster. Let $aX \geq \alpha$ denote a nontrivial valid inequality for RCut_n^K that is binding at all ratio-cut vectors for which $X_{12} \geq 0$ is satisfied tightly. We show that the two inequalities coincide up to a positive scaling, which by full dimensionality of RCut_n^K implies that $X_{12} \geq 0$ defines a facet of RCut_n^K .

Consider a partition of $[n]$ consisting of $K - 1$ nonempty clusters such that $\Gamma_1 = \{1, n\}$. Construct a second partition of $[n]$ consisting of K nonempty clusters obtained from the partition defined above by removing the n th point from the first cluster and putting it in the K th cluster. The corresponding ratio-cut vectors are binding and hence substituting in $aX = \alpha$ we obtain $a_{1n} = 0$.

Next for any $j \in [n] \setminus \{1, 2, n\}$ consider two partitions of $[n]$ consisting of K nonempty clusters corresponding to binding ratio-cut vectors, where in the first partition we have $\Gamma_1 = \{1, n\}$, $\Gamma_2 = \{j\}$ and $\cup_{k=3}^K \Gamma_k = [n] \setminus \{1, j, n\}$. The second partition is obtained from the first one by only modifying the first and second clusters as follows: $\Gamma_1 = \{1, j\}$, $\Gamma_2 = \{n\}$. Substituting the ratio-cut vectors in $aX = \alpha$ and using $a_{1n} = 0$ yields:

$$a_{1j} = 0, \quad \forall j \in [n] \setminus \{1, 2\}. \quad (21)$$

Similarly, for any $j \in [n] \setminus \{1, 2\}$ and for any $k \in [n] \setminus \{1, j\}$, consider two partitions of $[n]$ consisting of K nonempty clusters both of which correspond to binding ratio-cut

vectors, defined as follows: in the first partition we have $\Gamma_1 = \{1, j\}$, $\Gamma_2 = \{k\}$, and $\cup_{k=3}^K \Gamma_k = [n] \setminus \{1, j, k\}$. The second partition is obtained from the first one by only changing the first and second clusters as follows: $\Gamma_1 = \{1\}$, $\Gamma_2 = \{j, k\}$. Substituting the ratio-cut vectors in $aX = \alpha$ and using (21) yields

$$a_{jk} = 0, \quad \forall 2 \leq i < j \leq n.$$

Hence, since by assumption $aX \geq \alpha$ is nontrivial and valid for RCut_n^K we conclude that it can be equivalently written as $a_{12}X_{12} \geq 0$ where $a_{12} > 0$, implying that if $K \geq 3$ the inequality $X_{12} \geq 0$ defines a facet of RCut_n^K .

Now suppose that $K = 2$. We show that $X_{12} \geq 0$ is implied by a collection of inequalities all of which are valid for RCut_n^2 indicating that it is not facet-defining. Consider the following inequalities

$$2(X_{1i} + X_{2i}) + \sum_{j \in [n] \setminus \{1, 2, i\}} X_{ij} \leq 1 + X_{12}, \quad \forall i \in \{3, \dots, n\}. \quad (22)$$

By letting $S = \{1, 2, i\}$ for each $i \in \{3, \dots, n\}$, from Proposition 3 it follows that inequalities (22) are valid for RCut_n^2 . Moreover, take inequality $\sum_{1 \leq i < j \leq n} X_{ij} \geq (n-2)/2$ whose validity follows from Proposition 2; multiplying this inequality by -2 and adding the result to the inequality obtained by summing up all inequalities (22), we get $-nX_{12} \leq 0$. Hence $X_{ij} \geq 0$ does not define a facet of RCut_n^2 .

Finally, let us consider the polytope $\text{RCut}_n^{=K}$ for $3 \leq K \leq n-1$. In the above proof, with the exception of the first one, all of the defined ratio-cut vectors binding for $X_{ij} \geq 0$ correspond to K nonempty clusters and hence are present in $\text{RCut}_n^{=K}$. As $\text{RCut}_n^{=K}$ is a facet of RCut_n^K , it follows that the inequality $X_{ij} \geq 0$ defines a facet of $\text{RCut}_n^{=K}$ as well. \square

2.2 Connections with the cut polytope

The cut polytope, a celebrated polytope in combinatorial optimization, is the convex hull of all cut vectors of a graph (see [10] for an exposition). This polytope corresponds to the convex hull of the feasible region of the max-cut problem. Consider a graph with n nodes; we define a *cut vector* Y associated with a graph cut as follows: for any $1 \leq i < j \leq n$, let $Y_{ij} = 1$ if i and j are in the same partition and let $Y_{ij} = 0$, otherwise. The cut polytope Cut_n is then defined as the convex hull of all cut vectors. In this section, we describe some key similarities and differences between the cut polytope and the ratio-cut polytope.

The facial structure of the cut polytope has been extensively studied and numerous classes of facet-defining inequalities have been identified for this polytope. The most well-known class of facet-defining inequalities for Cut_n are *triangle inequalities* given by

$$Y_{ij} + Y_{ik} \leq 1 + Y_{jk}, \quad (23)$$

and

$$Y_{ij} + Y_{ik} + Y_{jk} \geq 1, \quad (24)$$

for all distinct $i, j, k \in [n]$ (see for example [10]).

Now let $l \in [n]$, and let $T \subseteq [n] \setminus \{l\}$ with $2 \leq |T| \leq K$; define $X_{ll} := 1 - \sum_{j \in [n] \setminus \{l\}} X_{lj}$. Then inequality (12) can be equivalently written as

$$\sum_{j \in T} X_{lj} \leq X_{ll} + \sum_{i, j \in T: i < j} X_{ij}. \quad (25)$$

By Proposition 3, inequalities of the form (25) define facets of RCut_n^K . Let $K = 2$; then all inequalities of the form (25) can be written as:

$$X_{ij} + X_{ik} \leq X_{ii} + X_{jk}, \quad \forall \text{ distinct } i, j, k \in [n], \quad (26)$$

where as before $X_{ii} := 1 - \sum_{j \in [n] \setminus \{i\}} X_{ij}$. Hence, inequalities (26) (and more generally, inequalities (25)) for the ratio-cut polytope can be considered as an equivalent of inequalities (23) for the cut polytope. Moreover, the fact-defining inequality (8) can be considered as an equivalent of inequalities (24) for the cut polytope. We further detail on some parallels between Cut_n and RCut_n^K in the next section as we introduce a relaxation of the ratio-cut polytope.

In spite of certain similarities, it is important to note that there are fundamental differences between the cut polytope and the ratio-cut polytope. For example, unlike the cut polytope, the ratio-cut polytope does not have the so-called “zero-lifting” property (see Section 26.5 of [10] for the definition of zero-lifting). Roughly speaking, the zero-lifting property implies that if an inequality defines a facet of Cut_n then it also defines a facet of $\text{Cut}_{n'}$ for all $n' > n$. Indeed, the lack of this property in case of inequalities (25) is hidden in the definition of X_{ii} .

2.3 A polyhedral relaxation of the ratio-cut polytope

We now define a polyhedral relaxation of RCut_n^K defined by all facet-defining inequalities given by Propositions 2, 3, and 4. We denote this relaxation by RMet_n^K due to its similarities to the *metric polytope*. The metric polytope defined by triangle inequalities (23) and (24) is a widely used relaxation of the cut polytope. Similarly, we define a polyhedral relaxation of RCut_n^K defined by equality (9) together with facet-defining inequalities given by Propositions 3, and 4. We denote this relaxation by $\text{RMet}_n^{=K}$. Notice that RMet_n^K is defined by a collection of inequalities all of which are facet-defining for RCut_n^K and $\text{RMet}_n^{=K}$ is the restriction of RMet_n^K to one of such inequalities. It then follows that $\text{RMet}_n^{=K}$ is a facet of RMet_n^K .

It is well-known that the metric polytope coincides with the cut polytope if and only if $n \leq 4$ [10]. The following demonstrates an analogous relation between RCut_n^K and RMet_n^K .

Proposition 5. $\text{RCut}_n^K = \text{RMet}_n^K$ if and only if $n \leq 4$.

Proof. If $n = 3$ and $K = \{2, 3\}$ or if $n = 4$ and $K \in \{2, 3, 4\}$, it can be checked, by direct calculation that the ratio-cut vectors constitute all vertices of RMet_n^K , implying $\text{RCut}_n^K = \text{RMet}_n^K$.

Now let $n \geq 5$ and consider some $K \in \{2, \dots, n\}$. To show that $\text{RCut}_n^K \subset \text{RMet}_n^K$, we present a point \bar{X} such that $\bar{X} \in \text{RMet}_n^K$ and $\bar{X} \notin \text{RCut}_n^K$. To prove the latter, we present an inequality that is valid for RCut_n^K but is violated by \bar{X} .

We first give the valid inequality for the ratio-cut polytope. Consider a pair $i, j \in [n]$ and let $T \subseteq [n] \setminus \{i, j\}$ with $|T| \geq 2$. Let $X_{ii} = 1 - \sum_{k \in [n] \setminus \{i\}} X_{ik}$ and suppose that X_{jj} is similarly defined. We first show that the inequality

$$\sum_{k \in T} (X_{ik} + X_{jk}) - X_{ij} \leq X_{ii} + X_{jj} + \sum_{k < l \in T} X_{kl} \quad (27)$$

is valid for RCut_n^K . Two cases arise:

- (i) i and j are in the same cluster of size Ω . Then $X_{ii} = X_{jj} = X_{ij} = \frac{1}{\Omega}$. Denote by ω the number of points in T that belong to the same cluster as i and j . Then $\sum_{k \in T} (X_{ik} + X_{jk}) = \frac{2\omega}{\Omega}$. Moreover, if $\omega \geq 2$, we have $\sum_{k < l \in T} X_{kl} \geq \binom{\omega}{2} \frac{1}{\Omega}$. Hence if $\omega \leq 1$, it suffices to show that $\frac{2\omega}{\Omega} - \frac{1}{\Omega} \leq \frac{1}{\Omega} + \frac{1}{\Omega}$ and if $\omega \geq 2$, it suffices to show that $\frac{2\omega}{\Omega} - \frac{1}{\Omega} \leq \frac{1}{\Omega} + \frac{1}{\Omega} + \binom{\omega}{2} \frac{1}{\Omega}$, both of which are valid.
- (ii) i and j are in two distinct clusters of size Ω_1 and Ω_2 , respectively. Then $X_{ii} = \frac{1}{\Omega_1}$, $X_{jj} = \frac{1}{\Omega_2}$ and $X_{ij} = 0$. Denote by ω_1 (resp. ω_2) the number of points in T that are in the same cluster with i (resp. j). Then $\sum_{k \in T} (X_{ik} + X_{jk}) = \frac{\omega_1}{\Omega_1} + \frac{\omega_2}{\Omega_2}$. Let $q_1 = \binom{\omega_1}{2}$ (resp. $q_2 = \binom{\omega_2}{2}$), if $\omega_1 \geq 2$ (resp. $\omega_2 \geq 2$) and let $q_1 = 0$ (resp. $q_2 = 0$), otherwise. Then it suffices to show that $\frac{\omega_1}{\Omega_1} + \frac{\omega_2}{\Omega_2} \leq \frac{1}{\Omega_1} + \frac{1}{\Omega_2} + \frac{q_1}{\Omega_1} + \frac{q_2}{\Omega_2}$. The validity of this statement follows from the fact that $\omega_1 \leq 1 + q_1$ and $\omega_2 \leq 1 + q_2$.

We now present a point $\bar{X} \in \text{RMet}_n^K$ that does not satisfy inequality (27). Suppose that $|T| = 3$; for notational simplicity, let $\{i, j\} = \{1, 2\}$ and $T = \{3, 4, 5\}$. Two cases arise:

- (i) $n = 5$: in this case, let

$$\begin{aligned}\bar{X}_{12} &= 0 \\ \bar{X}_{1k} = \bar{X}_{2k} &= \alpha = \frac{5}{24}, \quad k \in \{3, 4, 5\} \\ \bar{X}_{kl} &= \omega = \frac{2}{24}, \quad k < l \in \{3, 4, 5\}\end{aligned}$$

We now show that $\bar{X} \in \text{RMet}_5^K$. We have $\sum_{1 \leq i < j \leq 5} \bar{X}_{ij} = 6\alpha + 3\omega = \frac{3}{2} \geq \frac{5-K}{2}$, where the last inequality is valid for any $K \geq 2$; hence, inequality (8) is satisfied at \bar{X} . It remains to show the validity of inequalities (25) for $2 \leq |T| \leq \min\{K, 4\}$ and for $2 \leq K \leq 5$. We have $\bar{X}_{11} = \bar{X}_{22} = \beta = \frac{9}{24}$ and $\bar{X}_{kk} = \gamma = \frac{10}{24}$ for $k \in \{3, 4, 5\}$. Then for $|T| = 2$, it suffices to have $2\alpha \leq \beta + \omega$, $2\alpha \leq \gamma$, $\omega \leq \gamma$, all of which are valid. For $|T| = 3$, it suffices to have $3\alpha \leq \beta + 3\omega$ which is satisfied and all inequalities corresponding to $|T| = 4$ are implied by the above inequalities. Thus, we conclude that $\bar{X} \in \text{RMet}_5^K$. Substituting \bar{X} in inequality (27) yields $6\alpha - 0 \leq 2\beta + 3\omega$, which simplifies to $\frac{30}{24} \leq \frac{18}{24} + \frac{6}{24}$ and is clearly not valid.

- (ii) $n > 5$: in this case, let

$$\begin{aligned}\bar{X}_{12} &= 0 \\ \bar{X}_{1k} = \bar{X}_{2k} &= \alpha = \frac{n}{3(3n-7)}, \quad k \in \{3, 4, 5\} \\ \bar{X}_{kl} &= \omega = \frac{n}{6(3n-7)}, \quad k < l \in \{3, 4, 5\} \\ \bar{X}_{1k} = \bar{X}_{2k} &= \eta_1 = \frac{3n-14}{2(3n-7)(n-5)}, \quad k \in \{6, \dots, n\} \\ \bar{X}_{kl} &= \eta_2 = \frac{4n-21}{3(3n-7)(n-5)}, \quad k \in \{3, 4, 5\}, l \in \{6, \dots, n\} \\ \bar{X}_{kl} &= \eta_3 = \frac{3n-14}{(3n-7)(n-5)}, \quad k < l \in \{6, \dots, n\}.\end{aligned}$$

We now show that $\bar{X} \in \text{RMet}_n^K$. First, $\bar{X}_{ij} \geq 0$ for all $1 \leq i < j \leq n$. Moreover, $\sum_{1 \leq i < j \leq n} \bar{X}_{ij} = 6\alpha + 3\omega + 2(n-5)\eta_1 + 3(n-5)\eta_2 + \frac{(n-5)(n-6)}{2}\eta_3 = \frac{2n}{3n-7} + \frac{n}{2(3n-7)} +$

$\frac{3n-14}{3n-7} + \frac{4n-21}{3n-7} + \frac{(n-6)}{2} \frac{3n-14}{3n-7} = \frac{n-2}{2} \geq \frac{n-K}{2}$, implying inequality (8) is satisfied. We now establish the validity of inequalities (25) at \bar{X} , for $2 \leq |T| \leq K$. It can be checked that $\bar{X}_{11} = \bar{X}_{22} = \beta = \frac{n}{2(3n-7)}$ and $\bar{X}_{kk} = \gamma = \frac{2n}{3(3n-7)}$ for $k \in \{3, 4, 5\}$. From the construction of \bar{X} , it follows that the inequalities of the form (25) not implied by the rest are the following: $2\alpha \leq \beta + \omega$, $2\alpha \leq \gamma$, $\omega \leq \gamma$, $3\alpha \leq \beta + 3\omega$ all of which are satisfied by \bar{X} . Hence, $\bar{X} \in \text{RMet}_n^K$. Finally, substituting \bar{X} in inequality (27) yields $6\frac{n}{3(3n-7)} - 0 \leq 2\frac{n}{2(3n-7)} + 3\frac{n}{6(3n-7)}$, which simplifies to $2n \leq n + \frac{n}{2}$ and is clearly not valid. □

While for $n \geq 5$, the polytopes RMet_n^K and RCut_n^K do not coincide, next, we show that every ratio-cut vector is a vertex of RMet_n^K .

Proposition 6. *Every ratio-cut vector is a vertex of RMet_n^K and every ratio-cut vector corresponding to K nonempty clusters is a vertex of $\text{RMet}_n^{=K}$.*

Proof. We first show that every ratio-cut vector is a vertex of RMet_n^K . By Proposition 5 it suffices to consider $n \geq 5$. Let Γ_k , $k \in [K]$ form a partition of $[n]$, where as before we allow for some empty Γ_k . Denote by K' the number of nonempty clusters and denote by \hat{X} the corresponding ratio-cut vector. We show that \hat{X} is a vertex of RMet_n^K by presenting $\binom{n}{2}$ linearly independent facets of RMet_n^K that are satisfied tightly by \hat{X} . The following cases arise:

- (i) $K' = 1$: in this case for each i, j, k in the partition, consider facet-defining inequalities of the form (12) given by $2(X_{ij} + X_{ik}) + \sum_{l \in [n] \setminus \{j,k\}} X_{il} \leq 1 + X_{jk}$, $2(X_{ij} + X_{jk}) + \sum_{l \in [n] \setminus \{i,k\}} X_{jl} \leq 1 + X_{ik}$, and $2(X_{ik} + X_{jk}) + \sum_{l \in [n] \setminus \{i,j\}} X_{kl} \leq 1 + X_{ij}$.
- (ii) $K = K' = 2$: in this case for each i, j in one partition and for each k in the other partition consider facet-defining inequalities of the form (12) given by $2(X_{ij} + X_{ik}) + \sum_{l \in [n] \setminus \{j,k\}} X_{il} \leq 1 + X_{jk}$ and $2(X_{ij} + X_{jk}) + \sum_{l \in [n] \setminus \{i,k\}} X_{jl} \leq 1 + X_{ik}$. In addition, consider the facet defining inequality $\sum_{1 \leq i < j \leq n} X_{ij} \geq \frac{n}{2} - 1$.
- (iii) $K > 2$, $K' \neq 1$, in this case for each i, j in the same partition and for any k in a different partition consider facet-defining inequalities of the form (12) given by $2(X_{ij} + X_{ik}) + \sum_{l \in [n] \setminus \{j,k\}} X_{il} \leq 1 + X_{jk}$ and $2(X_{ij} + X_{jk}) + \sum_{l \in [n] \setminus \{i,k\}} X_{jl} \leq 1 + X_{ik}$. In addition, for each i, j not in the same partition consider the facet defining inequality $X_{ij} \geq 0$.

It can be checked that \hat{X} satisfies above inequalities tightly and that these inequalities contain $\binom{n}{2}$ linearly independent facets implying that \hat{X} is a vertex of RMet_n^K .

Finally, notice that every ratio-cut vector corresponding to K nonempty clusters belongs to $\text{RMet}_n^{=K}$ and by the above argument is a vertex of RMet_n^K . Moreover, $\text{RMet}_n^{=K}$ is a facet of RMet_n^K ; it then follows that all such ratio-cut vectors corresponding to K nonempty clusters are vertices of $\text{RMet}_n^{=K}$ as well. □

3 A new LP relaxation for K-means clustering

As we detailed in Section 2, the polytope $\text{RCut}_n^{=K}$ corresponds to a projection of the convex hull of the feasible region of Problem (3) defined by (7). Hence, to obtain an LP relaxation for K-means clustering, first, we outer-approximate the polytope $\text{RCut}_n^{=K}$ by

the polytope RMet_n^K . Next, we introduce additional variables $X_{ii} := 1 - \sum_{j \in [n] \setminus \{i\}} X_{ij}$ for all $i \in [n]$ and let $X_{ji} = X_{ij}$ for all $1 \leq i < j \leq n$. Let $t \in \{2, \dots, K\}$; for each $i \in [n]$ define $\mathcal{S}_i^t := \{S \subseteq [n] \setminus \{i\} : 2 \leq |S| \leq t\}$. It then follows that an LP relaxation of K-means clustering is given by:

$$\min \sum_{i,j \in [n]} d_{ij} X_{ij} \tag{LPK}$$

$$\text{s.t. } \text{Tr}(X) = K, \tag{28}$$

$$\sum_{j=1}^n X_{ij} = 1, \quad \forall i \in [n], \tag{29}$$

$$\sum_{j \in S} X_{ij} \leq X_{ii} + \sum_{j,k \in S: j < k} X_{jk}, \quad \forall i \in [n], \forall S \in \mathcal{S}_i^t, \tag{30}$$

$$X_{ij} \geq 0, \quad \forall 1 \leq i < j \leq n. \tag{31}$$

By the proof of Proposition 8, if $K = 2$, inequalities (31) are implied by equalities (28), (29) and inequalities (30). However, for $K \geq 3$, these inequalities are facet-defining and hence are present in Problem (LPK).

Clearly, letting $t = K$ results in the strongest LP relaxation. However, it is important to note that system (30) contains $\Theta(n^{t+1})$ inequalities and hence, for large t , Problem (LPK) is too expensive to solve. Indeed, even for $t = 2$, the above LP is expensive to solve for $n \geq 200$. To address this issue, a common approach is to devise a cutting plane generation scheme together with the dual Simplex algorithm to solve the LP in an iterative manner (see for example [19]). Given a fixed t , let us consider the separation problem over inequalities (30). For a fixed $i \in [n]$, these inequalities can be written as $\sum_{j,k \in S: j < k} X_{jk} \geq \sum_{j \in S} X_{ij} - X_{ii}$. Hence, the separation problem over these inequalities is quite similar to the separation problem over *clique inequalities* and therefore similar heuristics and acceleration techniques can be used (see for example [21]). We should also remark that inequalities of the form (30) corresponding to subsets S of smaller cardinality are *sparser* (i.e., contain fewer variables with nonzero coefficients) than those of the larger cardinality, a property that is highly desirable from a computational perspective. A careful selection of t and designing of an efficient cutting plane algorithm requires a systematic computational study and is a subject of future research. However, as we demonstrate in Section 5, the LP relaxation with $t = 2$ outperforms the SDP relaxation, even for $K = 5$ clusters.

Remark 1. Recall that Problem (6) is the existing LP relaxation for K-means clustering [4]. To show that the feasible region of Problem (LPK) is contained in the feasible region of this LP, it suffices to prove that inequalities $X_{ij} \leq X_{ii}$ for all $i \neq j \in [n]$ are implied by system (28)-(31). Without loss of generality consider $X_{12} \leq X_{11}$. Consider the following inequalities and equalities all of which are present in system (28)-(31):

$$(i) \quad X_{12} + X_{13} \leq X_{11} + X_{23},$$

$$(ii) \quad X_{12} + X_{23} \leq X_{22} + X_{13},$$

$$(iii) \quad X_{12} + X_{1j} \leq X_{11} + X_{2j}, \text{ for all } j \in \{4, \dots, n\},$$

$$(iv) \quad \sum_{j \in [n]} X_{1j} = 1,$$

$$(v) \sum_{j \in [n]} X_{2j} = 1.$$

Multiplying inequality (i) by +2, inequality (ii) by +1, each inequality of type (iii) by +1, equality (iv) by -1, equality (v) by +1 and adding all resulting inequalities and equalities yields $nX_{12} \leq nX_{11}$ and this completes the argument.

3.1 Optimality of the planted clusters

We now focus on the case with two clusters and obtain a sufficient condition under which the ratio-cut vector corresponding to a planted clustering is an optimal solution of the LP relaxation. As we discussed before, even with only two clusters, K-means clustering is NP-hard [6]. The LP relaxation of K-means clustering for $K = 2$ is given by:

$$\min \sum_{i,j \in [n]} d_{ij} X_{ij} \quad (\text{LP2})$$

$$\text{s.t. } \text{Tr}(X) = 2, \quad (32)$$

$$\sum_{j=1}^n X_{ij} = 1, \quad \forall 1 \leq i \leq n, \quad (33)$$

$$X_{ij} + X_{ik} \leq X_{ii} + X_{jk}, \quad \forall i \neq j \neq k \in [n], j < k, \quad (34)$$

where as before we let $X_{ji} = X_{ij}$ for all $1 \leq i < j \leq n$. We start by constructing the dual of Problem (LP2); define dual variables ω associated with (32), μ_i , $i \in [n]$ associated with (33), and λ_{ijk} for all $(i, j, k) \in \Omega := \{(i, j, k) : i \neq j \neq k \in [n], j < k\}$ associated with (34). It then follows that the dual of Problem (LP2) is given by

$$\max \quad - (2\omega + \sum_{i \in [n]} \mu_i)$$

$$\text{s.t. } \mu_i + \mu_j + \sum_{k \in [n] \setminus \{i, j\}} (\lambda_{ijk} + \lambda_{jik} - \lambda_{kij}) + 2d_{ij} = 0, \quad \forall 1 \leq i < j \leq n, \quad (35)$$

$$\omega + \mu_i - \sum_{\substack{j, k \in [n] \setminus \{i\}: \\ j < k}} \lambda_{ijk} = 0, \quad \forall i \in [n], \quad (36)$$

$$\lambda_{ijk} \geq 0, \quad \forall (i, j, k) \in \Omega,$$

where we let $\lambda_{ikj} = \lambda_{ijk}$ for all $(i, j, k) \in \Omega$. Now consider the following planted model: suppose that n is even, the first half of the points are in the first cluster and the second half are in the second cluster; define $\mathcal{C}_1 := \{1, \dots, n/2\}$ and $\mathcal{C}_2 := \{n/2 + 1, \dots, n\}$. Then the ratio-cut vector associated with this planted clustering is given by: $\bar{X}_{ij} = \frac{2}{n}$ for all $i < j \in \mathcal{C}_1$ and for all $i < j \in \mathcal{C}_2$ and $\bar{X}_{ij} = 0$, otherwise. We would like to obtain conditions under which \bar{X} is an optimal solution of Problem (LP2). To this end, it suffices to find a dual feasible point $(\bar{\lambda}, \bar{\mu}, \bar{\omega})$ for which strong duality is attained:

$$2\bar{\omega} + \sum_{i \in [n]} \bar{\mu}_i = -\frac{4}{n} \left(\sum_{i, j \in \mathcal{C}_1: i < j} d_{ij} + \sum_{i, j \in \mathcal{C}_2: i < j} d_{ij} \right). \quad (37)$$

For notational simplicity, for every $A \subseteq [n]$ and $f : A \rightarrow \mathbb{R}$, we define

$$\sum_{i \in A} f(i) := \frac{1}{|A|} \sum_{i \in A} f(i).$$

Moreover, for each $i \in \mathcal{C}_l$, $l \in \{1, 2\}$, let us define $d_i^{\text{in}} := \sum_{j \in \mathcal{C}_l} d_{ij}$, and $d_i^{\text{out}} := \sum_{j \in [n] \setminus \mathcal{C}_l} d_{ij}$.

We now present a sufficient condition for the optimality of the planted clusters.

Theorem 1. *Define*

$$\eta := \frac{1}{2} \left(\sum_{i \in \mathcal{C}_1} d_i^{\text{in}} + \sum_{i \in \mathcal{C}_2} d_i^{\text{in}} \right). \quad (38)$$

Then the ratio-cut vector corresponding to the planted clusters is an optimal solution of Problem (LP2) if for all $i, j \in \mathcal{C}_l$, $l \in \{1, 2\}$, we have

$$\sum_{k \in [n] \setminus \mathcal{C}_l} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} - d_{ij} \geq \eta. \quad (39)$$

Proof. By complementary slackness $\bar{\lambda}_{ijk} = 0$ if $i \in \mathcal{C}_1$ and $j, k \in \mathcal{C}_2$ or if $i \in \mathcal{C}_2$ and $j, k \in \mathcal{C}_1$. Substituting in (35) yields:

$$\bar{\mu}_i + \bar{\mu}_j + \sum_{k \notin \mathcal{C}_l} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik}) + \sum_{k \in \mathcal{C}_l \setminus \{i, j\}} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik} - \bar{\lambda}_{kij}) + 2d_{ij} = 0, \quad (40)$$

for every $i < j$ such that $i, j \in \mathcal{C}_l$, $l \in \{1, 2\}$ and

$$\bar{\mu}_i + \bar{\mu}_j + \sum_{k \in \mathcal{C}_1 \setminus \{i\}} (\bar{\lambda}_{ijk} - \bar{\lambda}_{kij}) + \sum_{k \in \mathcal{C}_2 \setminus \{j\}} (\bar{\lambda}_{jik} - \bar{\lambda}_{kij}) + 2d_{ij} = 0, \quad (41)$$

for every $i \in \mathcal{C}_1$, $j \in \mathcal{C}_2$. Moreover, equation (36) simplifies to

$$\bar{\omega} + \bar{\mu}_i - \sum_{\substack{j \in \mathcal{C}_l \setminus \{i\}, \\ k \notin \mathcal{C}_l}} \bar{\lambda}_{ijk} - \sum_{j < k \in \mathcal{C}_l \setminus \{i\}} \bar{\lambda}_{ijk} = 0, \quad (42)$$

for each $i \in \mathcal{C}_l$, $l \in \{1, 2\}$. Now for each $i, j \in \mathcal{C}_l$ and $k \notin \mathcal{C}_l$, $l \in \{1, 2\}$, let

$$\bar{\lambda}_{ijk} - \bar{\lambda}_{jik} = \frac{d_{jk} - d_{ik}}{n/2} + \frac{d_i^{\text{in}} - d_j^{\text{in}}}{n/2}. \quad (43)$$

Substituting (43) in (41) yields:

$$\bar{\mu}_i + \bar{\mu}_j + d_i^{\text{out}} + d_j^{\text{out}} + d_i^{\text{in}} + d_j^{\text{in}} - \sum_{k \in \mathcal{C}_1} d_k^{\text{in}} - \sum_{k \in \mathcal{C}_2} d_k^{\text{in}} = 0, \quad \forall i \in \mathcal{C}_1, j \in \mathcal{C}_2. \quad (44)$$

To satisfy (44), let

$$\bar{\mu}_i = -d_i^{\text{in}} - d_i^{\text{out}} + \eta, \quad \forall i \in [n]. \quad (45)$$

where η is defined by (38). Substituting (45) in (37) we obtain

$$\bar{\omega} = \frac{1}{2} \sum_{i \in [n]} (d_i^{\text{out}} - d_i^{\text{in}}). \quad (46)$$

Utilizing (43) and (45), equation (40) can be equivalently written as

$$\sum_{k \in \mathcal{C}_2} \bar{\lambda}_{ijk} + \frac{1}{2} \sum_{k \in \mathcal{C}_1 \setminus \{i, j\}} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik} - \bar{\lambda}_{kij}) = d_i^{\text{in}} - d_{ij} + d_j^{\text{out}} - \eta, \quad (47)$$

for any $(i, j) \in \mathcal{C}_1$. By (45) and (46), for each $i \in \mathcal{C}_1$, equation (42) simplifies to

$$\sum_{\substack{j \in \mathcal{C}_1 \setminus \{i\}, \\ k \in \mathcal{C}_2}} \bar{\lambda}_{ijk} + \sum_{j < k \in \mathcal{C}_1 \setminus \{i\}} \bar{\lambda}_{ijk} = \frac{1}{2} \sum_{j \in [n]} (d_j^{\text{out}} - d_j^{\text{in}}) - d_i^{\text{out}} - d_i^{\text{in}} + \eta. \quad (48)$$

We now obtain a set of conditions under which system (48) is implied by equalities (47). Firstly, it can be checked that

$$\sum_{j \neq k \in \mathcal{C}_1 \setminus \{i\}} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik} - \bar{\lambda}_{kij}) = 2 \sum_{j < k \in \mathcal{C}_1 \setminus \{i\}} \bar{\lambda}_{ijk}.$$

Hence, for each $i \in \mathcal{C}_1$ it suffices to have

$$\sum_{j \in \mathcal{C}_1 \setminus \{i\}} (d_i^{\text{in}} - d_{ij} + d_j^{\text{out}} - \eta) = \frac{1}{2} \sum_{j \in [n]} (d_j^{\text{out}} - d_j^{\text{in}}) - d_i^{\text{out}} - d_i^{\text{in}} + \eta,$$

whose validity can be verified by a simple calculation. Hence, to find a dual certificate, it suffices to find nonnegative $\bar{\lambda}_{ijk}$ satisfying equalities (40); that is, for each $(i, j) \in \mathcal{C}_1$, we should find $\bar{\lambda}_{ijk}$ satisfying the following system

$$\begin{aligned} \sum_{k \in \mathcal{C}_2} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik}) + \sum_{k \in \mathcal{C}_1 \setminus \{i, j\}} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik} - \bar{\lambda}_{kij}) &= d_i^{\text{out}} + d_j^{\text{out}} - 2d_{ij} + d_i^{\text{in}} + d_j^{\text{in}} - 2\eta \\ \bar{\lambda}_{ijk} \geq 0, \bar{\lambda}_{jik} \geq 0, \quad \forall k \in \mathcal{C}_2 \\ \bar{\lambda}_{ijk} - \bar{\lambda}_{jik} &= \frac{d_{jk} - d_{ik}}{n/2} + \frac{d_i^{\text{in}} - d_j^{\text{in}}}{n/2}, \quad \forall k \in \mathcal{C}_2 \\ \bar{\lambda}_{ijk} \geq 0, \bar{\lambda}_{jik} \geq 0, \bar{\lambda}_{kij} \geq 0, \quad \forall k \in \mathcal{C}_1 \setminus \{i, j\}. \end{aligned}$$

By letting $\bar{\lambda}_{ijk} \geq \max \left\{ 0, \frac{d_{jk} - d_{ik}}{n/2} + \frac{d_i^{\text{in}} - d_j^{\text{in}}}{n/2} \right\}$ and $\bar{\lambda}_{jik} \geq \max \left\{ 0, \frac{d_{ik} - d_{jk}}{n/2} + \frac{d_j^{\text{in}} - d_i^{\text{in}}}{n/2} \right\}$ for all $k \in \mathcal{C}_2$, it follows that the above system has a feasible solution, if

$$\frac{1}{2} \sum_{k \in \mathcal{C}_1 \setminus \{i, j\}} (\bar{\lambda}_{ijk} + \bar{\lambda}_{jik} - \bar{\lambda}_{kij}) \leq \sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} - d_{ij} - \eta, \quad (49)$$

for all $i, j \in \mathcal{C}_1$ together with nonnegativity of the remaining multipliers.

By letting $\bar{\lambda}_{ijk} = 0$ for all $i, j, k \in \mathcal{C}_l, l \in \{1, 2\}$, inequality (49) simplifies to condition (39) and this completes the proof. \square

As we demonstrate in Section 4, for the SBM, condition (39) leads to an overly conservative estimate for the minimum separation distance between cluster centers. We are hoping that the theoretical analysis presented in this paper serves as a starting point for deriving more realistic recovery guarantees for the proposed LP relaxation. Obtaining recovery guarantees for $K \geq 3$ is left for future research as well.

4 Recovery under the stochastic ball model

In this section, we consider a popular generative model for K-means clustering often referred to as the *stochastic ball model* in the literature. This random model is defined as follows: let $\{\gamma^k\}_{k \in [K]}$ be ball centers in \mathbb{R}^m . For each k , draw i.i.d. vectors $\{y^{k,i}\}_{i=1}^n$ from

some rotation-invariant distribution supported on the unit ball. The points in cluster k are then taken to be $x^{k,i} := y^{k,i} + \gamma^k$. Moreover, we define $\Delta := \min_{k \neq l \in [K]} \|\gamma^k - \gamma^l\|_2$.

Henceforth, we focus on the case of two clusters; throughout this section, whenever we say *with high probability*, we imply with probability tending to one as n tends to infinity. We are interested in the following question: what is the minimum separation distance Δ required for the LP relaxation to recover the planted clusters with high probability? Before proceeding further with addressing this question, we first establish a recovery threshold for K-means clustering under the SBM. This threshold then serves as a recovery limit for any convex relaxation of K-means clustering. In the following, we denote by $\{e_i\}_{i=1}^m$ the standard basis for \mathbb{R}^m . Moreover, for any $k \in [m]$, we denote by \mathcal{H}^k the k -dimensional Hausdorff measure.

4.1 Recovery for K-means clustering

In [6], the authors show that if the points are uniformly generated on two m -dimensional touching spheres for some $m \geq 3$, in the continuum limit, the K-means clustering problem identifies the two individual spheres as clusters. The goal of this section is to show that a similar recovery result is valid for the SBM.

We start by introducing some notation. We denote by $B(x, r)$ the closed m -dimensional ball centered at x with radius r . For a set $A \subset \mathbb{R}^m$, we denote by \bar{A} the closure of A and by ∂A the boundary of A . Given a Borel measure ρ on \mathbb{R}^m with support S and a Borel-measurable subset $S_1 \subset S$ with complement $S_2 = S \setminus S_1$, the *mean squared error* associated with the partition $\{S_1, S_2\}$ of S is

$$\mathcal{E}_S(S_1) = \min_{c \in \mathbb{R}^m} \int_{S_1} \|x - c\|^2 d\rho(x) + \min_{d \in \mathbb{R}^m} \int_{S_2} \|x - d\|^2 d\rho(x).$$

For every Borel subset $A \subset \mathbb{R}^m$ and every $k \in [m]$, we define the measure $\mathcal{H}^k \llcorner A$ as follows:

$$\mathcal{H}^k \llcorner A(B) = \mathcal{H}^k(A \cap B), \quad \text{for every Borel subset } B \subset \mathbb{R}^m.$$

For every Borel-measurable subset $A \subset \mathbb{R}^m$, we denote by $b(A) := \int_A x dx$ the barycenter of A . It is easy to check that, if A is a k -dimensional smooth set and $\mathcal{H}^k \llcorner A$ is a finite non-zero measure, then $b(A)$ is the only minimizer of the function $y \in \mathbb{R}^m \mapsto \int \|x - y\|^2 d\mathcal{H}^k \llcorner A$. In this section we prove the following result:

Theorem 2. *For any $m \geq 3$, let $S := B(-e_1, 1) \cup B(e_1, 1)$ and $\rho := \mathcal{H}^m \llcorner B(-e_1, 1) + \mathcal{H}^m \llcorner B(e_1, 1)$. Then, up to a set of zero Lebesgue measure, the partition $\{B(-e_1, 1), B(e_1, 1)\}$ of S is the unique minimizer of the mean squared error.*

In [6], the authors prove Theorem 2 in the case where ρ is the surface measure for the union of two touching spheres, i.e., $\rho = \mathcal{H}^{m-1} \llcorner \partial B(-e_1, 1) + \mathcal{H}^{m-1} \llcorner \partial B(e_1, 1)$. To this end, they first prove that an optimal partition is given by a separating hyperplane that is orthogonal to the symmetry axis (Lemma 3.5 and Theorem 2.2 in [6]). Subsequently, they examine the offset of the optimal separating hyperplane. More precisely they show the following:

Proposition 7. *[Theorems 2.4 and 2.5 in [6]] For any $m \geq 3$, let $S := \partial B(-e_1, 1) \cup \partial B(e_1, 1)$ and $\rho := \mathcal{H}^{m-1} \llcorner \partial B(-e_1, 1) + \mathcal{H}^{m-1} \llcorner \partial B(e_1, 1)$. Then the function $a \in \mathbb{R} \mapsto \mathcal{E}_S(\{x \in S : x_1 \leq -a\})$ attains a minimum at $a = 0$, and this minimum is unique.*

Remark 2. Proposition 7 is invariant under scaling. In particular if for any $r > 0$ we define $S := \partial B(-re_1, r) \cup \partial B(re_1, r)$ and $\rho := \mathcal{H}^{m-1} \llcorner \partial B(-re_1, r) + \mathcal{H}^{m-1} \llcorner \partial B(re_1, r)$, then the function $a \in \mathbb{R} \mapsto \mathcal{E}_S(\{x \in S : x_1 \leq -a\})$ attains a minimum at $a = 0$, and this minimum is unique. Moreover, in [6], the authors renormalize ρ to get a probability measure, but this changes $\mathcal{E}_S(S_1)$ just by a constant factor.

Since the proofs of Lemma 3.5 and Theorem 2.2 in [6] can be repeated verbatim for balls, in order to prove Theorem 2, we just need to prove the following analogous result to Proposition 7:

Proposition 8. For any $m \geq 3$, let $S := B(-e_1, 1) \cup B(e_1, 1)$ and $\rho := \mathcal{H}^m \llcorner B(-e_1, 1) + \mathcal{H}^m \llcorner B(e_1, 1)$. Then the function

$$a \in \mathbb{R} \mapsto F(a) := \mathcal{E}_S(\{x \in S : x_1 \leq -a\})$$

attains a minimum at $a = 0$, and this minimum is unique.

Proof. Assume by contradiction there exists $a \neq 0$ such that $F(a) \leq F(0)$. By symmetry, we can assume $a > 0$. Define $S_1 := \{x \in S : x_1 \leq -a\}$, $S_1^r := \{x \in \partial B(-e_1, r) : x_1 \leq -a\}$, $S_2^r := \{x \in \partial B(-e_1, r) : x_1 \geq -a\} \cup \partial B(e_1, r)$, and as before, we let $S_2 = S \setminus S_1$. Then, by Coarea formula (see Chapter 2 of [27])

$$\begin{aligned} & \int_0^1 \int_{\partial B(-e_1, r)} \|x + e_1\|^2 d\mathcal{H}^{m-1}(x) dr + \int_0^1 \int_{\partial B(e_1, r)} \|x - e_1\|^2 d\mathcal{H}^{m-1}(x) dr = F(0) \\ & \geq F(a) = \int_{S_1} \|x - b(S_1)\|^2 dx + \int_{S_2} \|x - b(S_2)\|^2 dx \\ & = \int_0^1 \int_{S_1^r} \|x - b(S_1)\|^2 d\mathcal{H}^{m-1}(x) dr + \int_0^1 \int_{S_2^r} \|x - b(S_2)\|^2 d\mathcal{H}^{m-1}(x) dr. \end{aligned}$$

We deduce that there exists $r \in (0, 1)$, such that

$$\begin{aligned} & \int_{\partial B(-e_1, r)} \|x + e_1\|^2 d\mathcal{H}^{m-1}(x) + \int_{\partial B(e_1, r)} \|x - e_1\|^2 d\mathcal{H}^{m-1}(x) \\ & \geq \int_{S_1^r} \|x - b(S_1)\|^2 d\mathcal{H}^{m-1}(x) + \int_{S_2^r} \|x - b(S_2)\|^2 d\mathcal{H}^{m-1}(x). \end{aligned} \tag{50}$$

Define $S_3^r := \{x \in \partial B(-e_1, r) : x_1 \geq -a\} \cup \partial B((2r-1)e_1, r)$. It then follows that

$$\begin{aligned} & \int_{S_1^r} \|x - b(S_1)\|^2 d\mathcal{H}^{m-1}(x) + \int_{S_2^r} \|x - b(S_2)\|^2 d\mathcal{H}^{m-1}(x) \\ & \geq \int_{S_1^r} \|x - b(S_1^r)\|^2 d\mathcal{H}^{m-1}(x) + \int_{S_3^r} \|x - b(S_3^r)\|^2 d\mathcal{H}^{m-1}(x) \\ & > \int_{\partial B(-e_1, r)} \|x + e_1\|^2 d\mathcal{H}^{m-1}(x) + \int_{\partial B((2r-1)e_1, r)} \|x - (2r-1)e_1\|^2 d\mathcal{H}^{m-1}(x) \\ & = \int_{\partial B(-e_1, r)} \|x + e_1\|^2 d\mathcal{H}^{m-1}(x) + \int_{\partial B(e_1, r)} \|x - e_1\|^2 d\mathcal{H}^{m-1}(x), \end{aligned} \tag{51}$$

where the first inequality follows from the definition of the barycenter and the second inequality follows from Proposition 7 and Remark 2. Combining (50) with (51), we get the desired contradiction. \square

Remark 3. *It is well-known that in dimension one, for both spheres and balls, K-means clustering recovers the planted clusters with high probability if and only if $\Delta > 1 + \sqrt{3}$ (see for example [14, 6]). In [6] the authors show that for two touching spheres in dimension two, the minimum of $F(a) = \mathcal{E}_S(\{x \in S : x_1 \leq -a\})$ is attained at a point $a \neq 0$. The authors of [14] numerically verify that a similar result holds for the SBM in dimension two. To date, the recovery threshold in dimension two, for both spheres and balls, remains an open question.*

4.2 Recovery for the LP relaxation

In this section, we obtain a recovery guarantee for the proposed LP relaxation under the SBM. Namely, we prove that our deterministic optimality condition given by inequality (39) implies that Problem (LP2) recovers the planted clusters with high probability, provided that $\Delta > 1 + \sqrt{3} \approx 2.73$. By Remark 3, this sufficient condition is tight if $m = 1$. This is a significant improvement compared to the only existing recovery result for an LP relaxation of K-means clustering stating that recovery is possible with high probability if and only if $\Delta > 4$ [4].

In the remainder of this section, for an event A , we denote by $\mathbb{P}(A)$ the probability of A . We denote by $\mathbb{E}[Y]$ the expected value of a random variable Y . In case of a multivariate random variable X_{ij} , the conditional expected value in j , with i fixed, will be denoted either with $\mathbb{E}_i[X]$ or with $\mathbb{E}^j[X]$. To prove the next theorem, we make use of two technical lemmas; to streamline the presentation, these lemmas are given in Section 6.

Theorem 3. *Let $K = 2$ and suppose that the points are generated according to the SBM. Then Problem (LP2) recovers the planted clusters with high probability, if $\Delta > 1 + \sqrt{3}$.*

Proof. To prove the statement, we need to show that for $\Delta > 1 + \sqrt{3}$, with high probability the ratio-cut vector corresponding to the planted clusters is the unique optimal solution of Problem (LP2).

To prove uniqueness, notice that the solution to the LP is not unique only if the objective function coefficient vector $d = \{d_{ij}\}_{1 \leq i < j \leq n}$ is orthogonal to an edge of the polytope $\text{RMet}_n^{=2}$. The objective function coefficient vector is generated from a probability distribution which is absolutely continuous with respect to the Lebesgue measure $\mathcal{H}^{\binom{n}{2}}$ in $\mathbb{R}^{\binom{n}{2}}$. The set of all “bad” directions however is the union of finitely many $\binom{n}{2} - 1$ -dimensional subspaces and hence is a zero $\mathcal{H}^{\binom{n}{2}}$ -measure set. Hence any optimal solution is unique with probability one.

We now address the question of optimality of the planted clusters under the SBM. In particular, we show that the optimality condition (39) holds with high probability. Namely, we show that, given $\epsilon > 0$ as defined in the statement of Lemma 1 (since $\Delta > 1 + \sqrt{3}$), we have

$$\begin{aligned} \mathbb{P} \left(\bigcap_{i,j \in \mathcal{C}_1} \left\{ d_{ij} + \eta - \sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} \leq 0 \right\} \right) \\ \geq 1 - \left(4e^{-2\binom{n/2}{2}\epsilon^2/16} + ne^{-n\epsilon^2/32} + 2\binom{n/2}{2}e^{-2n\epsilon^2/128} \right). \end{aligned}$$

We first observe that

$$\begin{aligned}
& \mathbb{P}(\{|\eta - \mathbb{E}[\eta]| \geq \epsilon\}) \\
&= \mathbb{P}\left(\left|\sum_{i,j \in \mathcal{C}_1} d_{ij} - \mathbb{E}\left[\sum_{i,j \in \mathcal{C}_1} d_{ij}\right] + \mathbb{E}\left[\sum_{i,j \in \mathcal{C}_2} d_{ij}\right] - \sum_{i,j \in \mathcal{C}_2} d_{ij}\right| \geq 2\epsilon\right) \\
&\leq \mathbb{P}\left(\left\{\left|\sum_{i,j \in \mathcal{C}_1} d_{ij} - \mathbb{E}\left[\sum_{i,j \in \mathcal{C}_1} d_{ij}\right]\right| \geq \epsilon\right\} \cup \left\{\left|\mathbb{E}\left[\sum_{i,j \in \mathcal{C}_2} d_{ij}\right] - \sum_{i,j \in \mathcal{C}_2} d_{ij}\right| \geq \epsilon\right\}\right) \\
&\leq \mathbb{P}\left(\left|\sum_{i,j \in \mathcal{C}_1} d_{ij} - \mathbb{E}\left[\sum_{i,j \in \mathcal{C}_1} d_{ij}\right]\right| \geq \epsilon\right) + \mathbb{P}\left(\left|\mathbb{E}\left[\sum_{i,j \in \mathcal{C}_2} d_{ij}\right] - \sum_{i,j \in \mathcal{C}_2} d_{ij}\right| \geq \epsilon\right) \\
&\leq 4e^{-2\binom{n/2}{2}\epsilon^2/16}.
\end{aligned} \tag{52}$$

The first inequality holds by set inclusion and the third inequality follows from Hoeffding's inequality (see for example Theorem 2.2.6 in [28]), since d_{ij} , $i, j \in \mathcal{C}_l$ are i.i.d. random variables for every $l \in \{1, 2\}$ and $d_{ij} \in [0, 4]$.

For notational simplicity, let us denote

$$t_{ij} := \mathbb{E}^k \left[\sum_{k \in \mathcal{C}_2} \min\{d_{ik} + \mathbb{E}_j[d_j^{\text{in}}], d_{jk} + \mathbb{E}_i[d_i^{\text{in}}]\} \right].$$

We now observe that

$$\begin{aligned}
& \mathbb{P}\left(\bigcup_{i,j \in \mathcal{C}_1} \left\{\left|t_{ij} - \mathbb{E}^k \left[\sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} \right]\right| \geq \epsilon\right\}\right) \\
&\leq \mathbb{P}\left(\bigcup_{i \in \mathcal{C}_1} \left\{\left|d_i^{\text{in}} - \mathbb{E}_i[d_i^{\text{in}}]\right| \geq \epsilon/2\right\}\right) \leq ne^{-n\epsilon^2/32},
\end{aligned} \tag{53}$$

where the first inequality follows from the linearity of expectation and the second inequality follows from the application of Hoeffding's inequality and taking the union bound. Combining the previous estimates, we conclude the claimed inequality:

$$\begin{aligned}
& \mathbb{P}\left(\bigcap_{i,j \in \mathcal{C}_1} \left\{d_{ij} + \eta - \sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} \leq 0\right\}\right) \\
&\geq \mathbb{P}\left(\bigcap_{i,j \in \mathcal{C}_1} \left\{d_{ij} + \eta - d_{ij} - \mathbb{E}[\eta] + t_{ij} - \sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} \leq 3\epsilon\right\}\right) \\
&\geq \mathbb{P}\left(\left\{|\eta - \mathbb{E}[\eta]| < \epsilon\right\} \cap \bigcap_{i,j \in \mathcal{C}_1} \left\{\left|t_{ij} - \mathbb{E}^k \left[\sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} \right]\right| < \epsilon\right\}\right) \\
&\cap \bigcap_{i,j \in \mathcal{C}_1} \left\{\left|\mathbb{E}^k \left[\sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\} \right] - \sum_{k \in \mathcal{C}_2} \min\{d_{ik} + d_j^{\text{in}}, d_{jk} + d_i^{\text{in}}\}\right| < \epsilon\right\} \\
&\geq 1 - \left(4e^{-2\binom{n/2}{2}\epsilon^2/16} + ne^{-n\epsilon^2/32} + 2\binom{n/2}{2}e^{-2n\epsilon^2/128}\right).
\end{aligned}$$

The first inequality follows from Lemma 1, since $\Delta > 1 + \sqrt{3}$; the second inequality holds by set inclusion; the third inequality is obtained by taking the union bound, followed by the application of Hoeffding's inequality, inequalities (52) and (53). \square

5 Numerical Experiments

In this section, we conduct a preliminary numerical study to demonstrate the desirable numerical properties of the proposed LP relaxation defined by (LPK). A comprehensive

computational study including the design and implementation of a separation algorithm for inequalities (30) is a subject of future research. First, we compare the recovery properties of the proposed LP relaxation versus the SDP relaxation defined by (5). To this end, we set $m \in \{2, 3\}$, $K \in \{2, 3\}$ and generate the points in each cluster according to the SBM. We set $t = 2$ in the LP relaxation. As before we denote by Δ the minimum distance between the cluster centers. For each fixed configuration (m, K) , we consider various values for Δ ; namely, we set $\Delta \in [2 : 0.01 : \bar{\Delta}]$, where $\bar{\Delta}$ is set to a value at which recovery is clearly achieved for both algorithms. For each fixed Δ , we conduct 20 random trials. We count the number of times the optimization algorithm returns the planted clusters as the optimal solution; dividing this number by total number of trials, we obtain the empirical rate of success. All experiments are performed on the NEOS server [7]; LPs are solved with GAMS/CPLEX [13] and SDPs are solved with GAMS/MOSEK [1].

Our results are depicted in Figure 2. As can be seen from these graphs, in all configurations, the LP clearly outperforms the SDP in recovering the planted clusters. In particular, results for $K = 2$ suggest that our recovery guarantee of Section 4 is excessively conservative. In addition, it can be seen that the recovery threshold of the LP relaxation in dimension $m = 3$ is better than the threshold in dimension $m = 2$; this effect is not reflected in our recovery guarantee and is a subject to future research. We also remark that in all these experiments, the optimal solution of the LP is a partition matrix; that is, even when the LP fails in recovering the planted clusters, its optimal solution is still a partition matrix and hence optimal for the original nonconvex problem. This is in sharp contrast with the SDP relaxation whose solution is not a partition matrix whenever it fails in recovering the planted clusters.

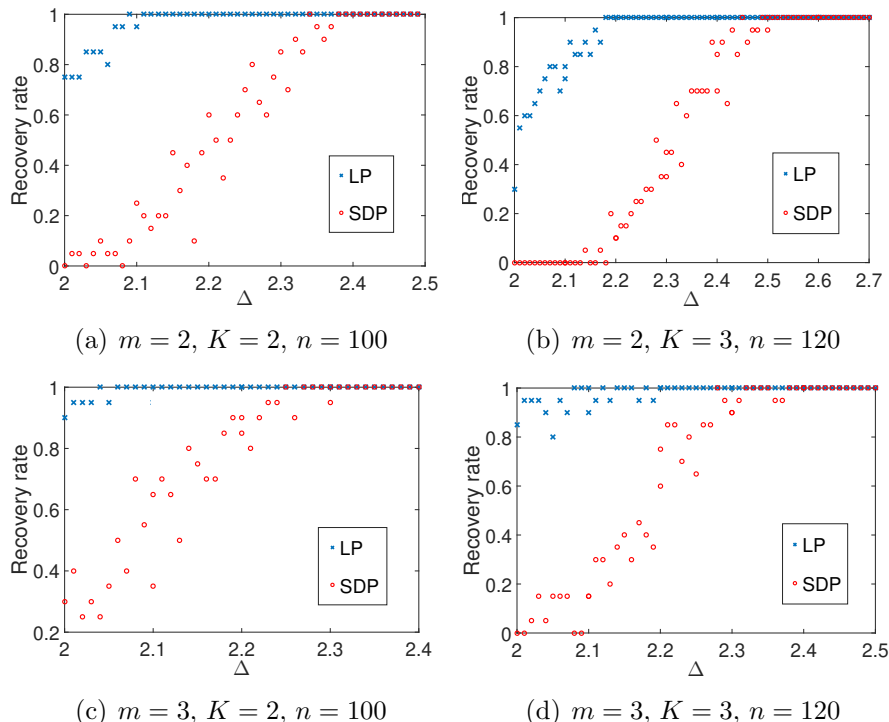


Figure 2: The empirical probability of success of the LP versus the SDP in recovering the planted clusters when the points are generated according to the SBM.

In all above experiments, we set $t = 2$; this implies that in cases with $K \geq 3$, the LP relaxation can be further strengthened by adding inequalities of the form (30)

corresponding to subsets S with $|S| > 2$. However, such a strengthening implies a significantly higher cost for the LP relaxation and requires the implementation of a clever separation algorithm. We now show that even for $K > 3$, the weakest LP relaxation, i.e., Problem (LPK) with $t = 2$, outperforms the SDP relaxation. To this end, we set $m = 2$ and let $K \in \{4, 5\}$; the points in each cluster are generated according to the SBM and the cluster centers have a hive-shaped geometry (see Figure 3). As before, we set $\Delta \in [2 : 0.01 : \bar{\Delta}]$ and for each fixed Δ , we conduct 20 random trials. Our results are depicted in Figure 4. As can be seen from these graphs, the weakest LP relaxation outperforms the SDP relaxation for both $K = 4$ and $K = 5$ clusters.

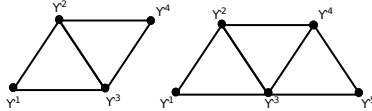


Figure 3: Cluster centers $\gamma^k, k \in [K]$ with hive-shaped geometry. The parameter Δ is defined as the distance between two adjacent centers.

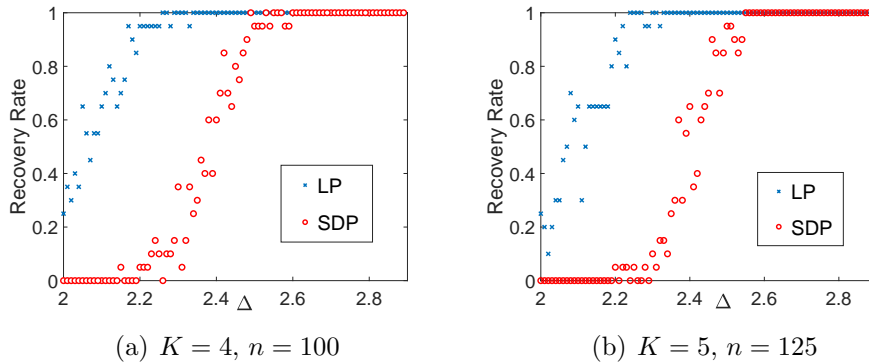


Figure 4: The empirical probability of success of the weakest LP versus the SDP in recovering planted clusters for the SBM in dimension two, with $K = 4$ clusters (Figure 4(a)) and with $K = 5$ clusters (Figure 4(b)).

We now illustrate the impact of inequalities (30) on the quality of the LP relaxation via a simple numerical experiment. As we mentioned before, a careful selection of parameter t requires the development of a separation algorithm that is beyond the scope of this paper. We consider two LP relaxations of K-means clustering: (i) Problem (LPK) with $t = 2$, referred to as LPt2 and (ii) Problem (LPK) with $t = 3$, referred to as LPt3. As before, we set $m = 2$ and we generate the points according to the SBM. We consider $K \in \{4, 5\}$ where the cluster centers are chosen as shown in Figure 3. To better understand the impact of inequalities (30), in addition to recovery, we compare the *tightness* of the two LPs. That is, we say that a relaxation is tight, if the returned optimal solution is a partition matrix as defined by (2). Moreover, we assume that the balls from which the points are drawn may overlap; that is, we let $\Delta \in [0 : 0.1 : \bar{\Delta}]$ and for each fixed Δ we conduct 50 random trials. Indeed in practice, there is often no clear separation between the underlying clusters, and the recovery question does not make much sense; in such settings, one is interested in finding an optimal clustering (i.e., an optimal partition matrix) which may or may not correspond to a planted clustering.

Our results are depicted in Figure 5. Interestingly, while LPt2 and LPt3 have identical performance with respect to recovery, the addition of inequalities (30) with $|S| = 3$,

clearly improves the tightness of the LP relaxation. This serves as a strong motivation for developing an efficient separation algorithm for inequalities (30). We conclude by acknowledging that in order to fully investigate the relative computational benefits of the LP relaxation versus the SDP relaxation for K-means clustering, a comprehensive numerical study on various real data sets is needed. This is indeed a subject of future research.

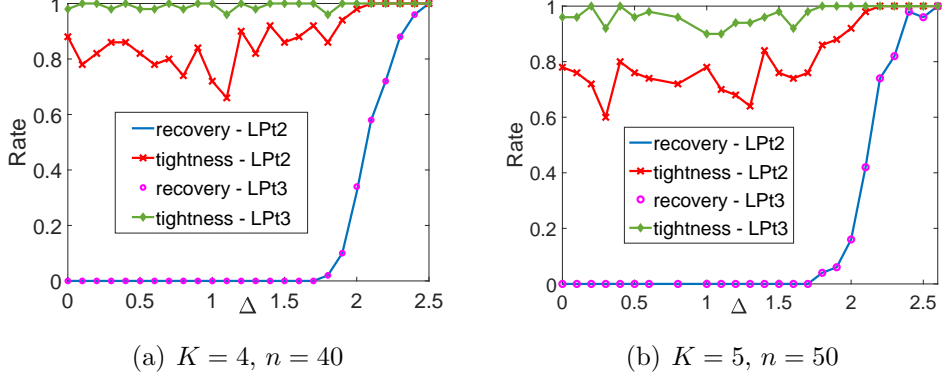


Figure 5: Comparing the quality of two LP relaxations, LPT2 vs LPT3 for the SBM in dimension two, with $K = 4$ clusters (Figure 5(a)) and with $K = 5$ clusters (Figure 5(b)).

6 Technical proofs

In this section, we present the two technical lemmas that we utilized to prove Theorem 3. In the following, for a Borel set $A \subset \mathbb{R}^m$ and measurable function $f : \mathbb{R}^m \rightarrow \mathbb{R}$, we define

$$\int_A f(x) d\mathcal{H}^m(x) := \frac{1}{\mathcal{H}^m(A)} \int_A f(x) d\mathcal{H}^m(x).$$

Moreover, for any $x \in \mathbb{R}^m$, we denote by x_i the i th component of x . Given two points $x, y \in \mathbb{R}^m$, the notation $x \parallel y$ means that x and y are linearly dependent.

Lemma 1. *Suppose that the random points are generated according to the SBM. Then the following inequality holds provided that $\Delta > 1 + \sqrt{3}$:*

$$\epsilon := \frac{1}{3} \left(\inf_{i,j \in \mathcal{C}_1} \mathbb{E}^k \left[\sum_{k \in \mathcal{C}_2} \min\{d_{ik} + \mathbb{E}_j[d_j^{in}], d_{jk} + \mathbb{E}_i[d_i^{in}]\} \right] - d_{ij} - \mathbb{E}[\eta] \right) > 0. \quad (54)$$

Proof. Denote by \mathcal{B}_1 and \mathcal{B}_2 the balls corresponding to the first and second clusters, respectively. Up to a rotation we can assume that the center of \mathcal{B}_1 and \mathcal{B}_2 are 0 and Δe_1 , respectively. For notational simplicity, we denote the i th (resp. j th) point in \mathcal{B}_1 by x (resp. y). By Lemma 2, it suffices to show that inequality (54) can be equivalently written as:

$$\max_{x,y \in \mathcal{B}_1} \int_{\mathcal{B}_2} \max\{x^T z, y^T z\} d\mathcal{H}^m(z) - x^T y < \frac{1}{2} \Delta^2. \quad (55)$$

First, notice that for any $i \in \mathcal{B}_1$ we have

$$\begin{aligned} \mathbb{E}_i[d_i^{in}] &= \int_{\mathcal{B}_1} \|x - z\|^2 d\mathcal{H}^m(z) = \|x\|^2 + \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z) - 2x^T \int_{\mathcal{B}_1} z d\mathcal{H}^m(z) \\ &= \|x\|^2 + \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z). \end{aligned} \quad (56)$$

By symmetry, the same calculation holds for $\mathbb{E}_i[d_i^{\text{in}}]$ with $i \in \mathcal{B}_2$. By (56), we have

$$\begin{aligned} \mathbb{E} \left[\sum_{k \in \mathcal{B}_1} d_k^{\text{in}} \right] &= \mathbb{E} \left[\sum_{k \in \mathcal{B}_2} d_k^{\text{in}} \right] \\ &= \int_{\mathcal{B}_1} \left(\|z\|^2 + \int_{\mathcal{B}_1} \|w\|^2 d\mathcal{H}^m(w) \right) d\mathcal{H}^m(z) = 2 \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z). \end{aligned} \quad (57)$$

Hence, by (56) and (57), inequality (54) reads

$$\min_{x, y \in \mathcal{B}_1} \int_{\mathcal{B}_2} \min\{\|x - z\|^2 + \|y\|^2, \|y - z\|^2 + \|x\|^2\} d\mathcal{H}^m(z) - \|x - y\|^2 > \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z),$$

which expanding the squares gives

$$\min_{x, y \in \mathcal{B}_1} \int_{\mathcal{B}_2} \|z\|^2 + \min\{-2x^T z, -2y^T z\} d\mathcal{H}^m(z) + 2x^T y > \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z). \quad (58)$$

Via a change of variables

$$\begin{aligned} \int_{\mathcal{B}_2} \|z\|^2 d\mathcal{H}^m(z) &= \int_{\mathcal{B}_1} \|\Delta e_1 + z\|^2 d\mathcal{H}^m(z) = \int_{\mathcal{B}_1} \|\Delta e_1\|^2 + \|z\|^2 + 2\Delta e_1^T z d\mathcal{H}^m(z) \\ &= \Delta^2 + \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z) + 2\Delta e_1^T \int_{\mathcal{B}_1} z d\mathcal{H}^m(z) = \Delta^2 + \int_{\mathcal{B}_1} \|z\|^2 d\mathcal{H}^m(z), \end{aligned}$$

hence (58) reads

$$\min_{x, y \in \mathcal{B}_1} \int_{\mathcal{B}_2} \min\{-2x^T z, -2y^T z\} d\mathcal{H}^m(z) + 2x^T y > -\Delta^2,$$

which is equivalent to (55). □

Lemma 2. *Inequality (55) holds if and only if $\Delta > 1 + \sqrt{3}$.*

Proof. We will prove that the maximum of the left-hand side of inequality (55) over all $x, y \in \mathcal{B}_1$ is attained at $(e_1, -e_1)$. This in turn implies that inequality (55) is satisfied if and only if

$$\Delta + 1 = \int_{\mathcal{B}_2} z_1 d\mathcal{H}^m(z) + 1 < \frac{1}{2} \Delta^2,$$

which is true if and only if $\Delta > 1 + \sqrt{3}$; i.e., the desired condition.

Define

$$F(x, y) := \int_{\mathcal{B}_2} \max\{x^T z, y^T z\} - x^T y d\mathcal{H}^m(z).$$

Our goal is to show that

$$\max_{x, y \in \mathcal{B}_1} F(x, y) = F(e_1, -e_1). \quad (59)$$

We divide the proof in several steps:

Step 1. Slicing:

Let z, w be any pair of points in \mathcal{B}_2 satisfying $z_1 = w_1, z_2 = -w_2 \geq 0, z_j = w_j = 0$ for all $j \in \{3, \dots, m\}$. Define

$$H(x, y) := \left\{ \frac{1}{2} \max\{x^T z, y^T z\} + \frac{1}{2} \max\{x^T w, y^T w\} - x^T y \right\}.$$

Then (59) holds if the following holds

$$\max_{x,y \in \mathcal{B}_1} H(x,y) = H(e_1, -e_1). \quad (60)$$

Proof of Step 1. Since

$$F(x,y) = \frac{1}{\mathcal{H}^m(\mathcal{B}_2)} \int_{\Delta-1}^{\Delta+1} \int_{\{z_1=s\} \cap \mathcal{B}_2} \max\{x^T z, y^T z\} - x^T y d\mathcal{H}^{m-1}(z) ds,$$

to show (59) it is enough to show that the function

$$G(x,y) := \int_{\{z_1=s\} \cap \mathcal{B}_2} \max\{x^T z, y^T z\} - x^T y d\mathcal{H}^{m-1}(z)$$

is maximized in $x = e_1, y = -e_1$, for every $s \in [\Delta - 1, \Delta + 1]$. Denoting $A := \{z_1 = s, z_2 \geq 0\} \cap \mathcal{B}_2$, then

$$G(x,y) = \int_A \frac{1}{2} \max\{x^T z, y^T z\} + \frac{1}{2} \max\{x^T(2se_1 - z), y^T(2se_1 - z)\} - x^T y d\mathcal{H}^{m-1}(z).$$

Hence, it is enough to prove that for every $s \in [\Delta - 1, \Delta + 1]$ and for every $z \in A$,

$$\max_{x,y \in \mathcal{B}_1} \left\{ \frac{1}{2} \max\{x^T z, y^T z\} + \frac{1}{2} \max\{x^T(2se_1 - z), y^T(2se_1 - z)\} - x^T y \right\}, \quad (61)$$

is achieved at $(e_1, -e_1)$. Since Problem (61) is invariant under a rotation of the space around the axis generated by e_1 , we conclude that solving Problem (61) is equivalent to solving Problem (60).

Step 2. *Symmetric distribution of the maxima:*

Let z, w be any pair of points as defined in Step 1. Define

$$I(x,y) := \frac{1}{2} x^T z + \frac{1}{2} y^T w - x^T y.$$

In order to show that (60) holds, it suffices to prove that

$$\max_{\substack{x,y \in \mathcal{B}_1 \\ x^T z \geq y^T z, y^T w \geq x^T w}} \{I(x,y)\} \leq H(e_1, -e_1) = z_1 + 1. \quad (62)$$

Proof of Step 2. Assume by contradiction that (62) holds, but (60) does not hold. Then there exists $z, w \in \mathcal{B}_2, z_1 = w_1, z_2 = -w_2$ and $z_j = w_j = 0$ for all $j \in \{3, \dots, m\}$ and $\bar{x}, \bar{y} \in \mathcal{B}_1$ such that $\bar{x}^T z \geq \bar{y}^T z, \bar{x}^T w \geq \bar{y}^T w$ and $H(\bar{x}, \bar{y}) > H(e_1, -e_1)$. We deduce that

$$\begin{aligned} H(e_1, -e_1) &< H(\bar{x}, \bar{y}) = \frac{1}{2} \bar{x}^T z + \frac{1}{2} \bar{x}^T w - \bar{x}^T \bar{y} \leq \max_{x,y \in \mathcal{B}_1} \frac{1}{2} x^T z + \frac{1}{2} x^T w - x^T y \\ &= \max_{x \in \mathcal{B}_1} \frac{1}{2} x^T z + \frac{1}{2} x^T w + \|x\|. \end{aligned} \quad (63)$$

Since the function $\frac{1}{2} x^T z + \frac{1}{2} x^T w + \|x\|$ is convex in x , then

$$\max_{x \in \mathcal{B}_1} \frac{1}{2} x^T z + \frac{1}{2} x^T w + \|x\| = \max_{x \in \partial \mathcal{B}_1} \frac{1}{2} x^T z + \frac{1}{2} x^T w + \|x\| = \max_{x \in \partial \mathcal{B}_1} \frac{1}{2} x^T z + \frac{1}{2} x^T w + 1. \quad (64)$$

The maximization problem on the right hand side of (64) has critical points satisfying

$$z + w + 2\lambda x = 0. \quad (65)$$

Since $z, w \in \mathcal{B}_2$, $z_1 = w_1$, $z_2 = -w_2 \geq 0$ and $z_j = w_j = 0$ for every $j = 3, \dots, m$, then equation (65) implies that $x \parallel e_1$. We deduce that any maximum point of (64) satisfies $x = te_1$, with $t \in [-1, 1]$:

$$\max_{x \in \partial \mathcal{B}_1} \frac{1}{2} x^T z + \frac{1}{2} x^T w + 1 = \max_{t \in [-1, 1]} tz_1 + 1, \quad (66)$$

and the maximum point of (66) is attained at $t = 1$, since $z_1 > 0$. Combining (63), (64) and (66), we deduce the contradiction $H(e_1, -e_1) < z_1 + 1 = H(e_1, -e_1)$.

Step 3. *Reduction from balls to disks:*

To show the validity of (62), we can restrict to dimension $m = 2$.

Proof of Step 3. We fix $z = (z_1, z_2, 0, \dots, 0)$ and $w = (z_1, -z_2, 0, \dots, 0)$. Denote $x = (x_1, x')$ and $y = (y_1, y')$, where $x' := (x_2, \dots, x_m)$ and $y' := (y_2, \dots, y_m)$. We will use the same notation also for z, w . Moreover denote $\tilde{x} = (x_1, \tilde{x}')$ and $\tilde{y} = (y_1, \tilde{y}')$, where $\tilde{x}' := (\tilde{x}_2, 0, \dots, 0)$, $\tilde{y}' := (\tilde{y}_2, 0, \dots, 0)$, such that $\|x'\| = \|\tilde{x}'\|$ and $\|y'\| = \|\tilde{y}'\|$, $\tilde{x}_2 \geq 0$ and $\tilde{y}_2 \leq 0$. To prove the claim, it suffices to show that the maximum in (62) is attained at $x, y \in \text{span}\{e_1, e_2\}$. To this end, it is enough to show that $I(x, y) \leq I(\tilde{x}, \tilde{y})$, which is equivalent to

$$\frac{1}{2}(x')^T z' + \frac{1}{2}(y')^T w' - (x')^T y' \leq \frac{1}{2}(\tilde{x}')^T z' + \frac{1}{2}(\tilde{y}')^T w' - (\tilde{x}')^T \tilde{y}'.$$

In turn, this inequality is valid because

- (i) by definition $\tilde{x}' \parallel z'$, $\tilde{y}' \parallel w'$, $\tilde{x}_2 \geq 0$, $\tilde{y}_2 \leq 0$ and $z_2 \geq 0$; then we have $(x')^T z' \leq (\tilde{x}')^T z'$ and $(y')^T w' \leq (\tilde{y}')^T w'$.
- (ii) by definition $\|x'\| = \|\tilde{x}'\|$, $\|y'\| = \|\tilde{y}'\|$, $\tilde{x}_2 \geq 0$, $\tilde{y}_2 \leq 0$, and $\tilde{x}' \parallel \tilde{y}'$; then we have $(x')^T y' \geq (\tilde{x}')^T \tilde{y}'$.

Step 4. *Reduction from disks to circles:*

In order to prove Problem (62), it is enough to show that

$$\max_{\substack{x, y \in \partial \mathcal{B}_1 \\ x^T z \geq y^T z, y^T w \geq x^T w}} I(x, y) \leq H(e_1, -e_1) = z_1 + 1, \quad (67)$$

for every $z \in \mathcal{B}_2$, $z_1 = w_1$ and $z_2 = -w_2 \geq 0$.

Proof of Step 4. Fix $x, y \in \mathcal{B}_1$. To prove this step, it is enough to find $x', y' \in \partial \mathcal{B}_1$ such that $I(x', y') \geq I(x, y)$. Let us denote $\bar{x} = x/\|x\|$ if $x \neq 0$ and $\bar{x} = e_1$ if $x = 0$. Let us denote $\bar{y} = y/\|y\|$ if $y \neq 0$ and $\bar{y} = e_1$ if $y = 0$. Since x, y, z, w are fixed, we define the constants $a = \frac{1}{2}\bar{x}^T z$, $b = \frac{1}{2}\bar{y}^T w$ and $c = \bar{x}^T \bar{y}$. We consider the problem

$$\max_{(r_1, r_2) \in [-1, 1]^2} I(r_1 \bar{x}, r_2 \bar{y}) = \max_{(r_1, r_2) \in [-1, 1]^2} r_1 a + r_2 b - r_1 r_2 c.$$

It is well-known that the maximum of a bilinear function over a box is attained at a vertex of the box and this completes the proof.

Step 5. *Symmetric local maxima:*

For any pair $x, y \in \partial\mathcal{B}_1$ of the form $x_1 = y_1$ and $x_2 = -y_2$, we have

$$I(x, y) \leq H(e_1, -e_1).$$

Proof of Step 5. Given such symmetric pair (x, y) , the objective function evaluates to $I(x, y) = z_1x_1 + z_2x_2 - x_1^2 + x_2^2$. Using $x_1^2 + x_2^2 = 1$ and $z_2\sqrt{1-x_1^2} \leq z_2$, it suffices to show that

$$z_2 \leq 2x_1^2 - z_1x_1 + z_1, \quad \forall x_1 \in [-1, 1]. \quad (68)$$

Since the function $\hat{f}(x_1) := 2x_1^2 - z_1x_1 + z_1$ on the right hand side of (68) is a convex parabola in x_1 , its minimum is either attained at one of the end points or at $\tilde{x}_1 = \frac{z_1}{4}$, provided that $-1 \leq \frac{z_1}{4} \leq 1$. Since $\Delta - 1 \leq z_1 \leq \Delta + 1$, the point \tilde{x}_1 lies in the domain only if $\Delta - 1 \leq z_1 \leq \min\{4, \Delta + 1\}$. The value of \hat{f} at $x_1 = -1$ and $x_1 = 1$ evaluates to $2 + 2z_1$ and 2 , respectively, both of which are bigger than z_2 . Hence it remains to show that

$$\sqrt{1-u^2} \leq (u+\Delta) - \frac{(u+\Delta)^2}{8}, \quad -1 \leq u \leq \min\{4-\Delta, 1\},$$

where we set $u := z_1 - \Delta$ and we use that $z_2 \leq \sqrt{1-u^2}$. Since $u + \Delta \leq 4$, the right hand side of the above inequality is increasing in Δ ; hence it suffices to show its validity at $\Delta = 2$; i.e.,

$$\sqrt{1-u^2} \leq (u+2) - \frac{(u+2)^2}{8}, \quad -1 \leq u \leq 1.$$

The right-hand side of the above inequality is concave and hence is lower bounded by its secant line through the boundary points $(-1, 7/8)$, $(1, 15/8)$; hence it suffices to show that $\sqrt{1-u^2} \leq \frac{1}{2}(u + \frac{11}{4})$ for all $-1 \leq u \leq 1$. Squaring both sides and rearranging the terms, the above inequality can be equivalently written as $u^2 + \frac{11}{10}u + \frac{57}{80} \geq 0$, where $-1 \leq u \leq 1$. It can be shown that the minimum of the left hand side of this inequality is attained at $u = -\frac{11}{20}$ and is equal to 0.41 and this completes the proof.

Step 6. Decomposition of the circle:

To solve Problem (67), it suffices to solve

$$\max_{\substack{x, y \in \partial\mathcal{B}_1 \cap \{x_1 \leq 0, y_1 \geq 0\} \\ x^T z \geq y^T z, y^T w \geq x^T w}} I(x, y) \leq H(e_1, -e_1) = z_1 + 1, \quad (69)$$

for every $z \in \mathcal{B}_2$, $z_1 = w_1$, $z_2 = -w_2 \geq 0$.

Proof of Step 6. We first consider the case when $x_1 \leq 0$ and $y_1 \leq 0$. Since $z_1 > 0$, then $x_1z_1 \leq -x_1z_1$, $y_1z_1 \leq -y_1z_1$. We deduce that $I(x, y) \leq I((-x_1, x_2), (-y_1, y_2))$.

Now, since the case $\{x_1 \geq 0, y_1 \leq 0\}$ is symmetric to the case $\{x_1 \leq 0, y_1 \geq 0\}$, we just need to show that

$$\max_{\substack{x, y \in \partial\mathcal{B}_1 \cap \{x_1 \geq 0, y_1 \geq 0\} \\ x^T z \geq y^T z, y^T w \geq x^T w}} I(x, y) \leq H(e_1, -e_1) = z_1 + 1.$$

Consider $x, y \in \partial\mathcal{B}_1$ such that $x_1 \geq 0$, $y_1 \geq 0$, $x^T z \geq y^T z$, $y^T w \geq x^T w$. If x_2, y_2 are both negative (resp. both positive), we can consider the new couple $(x_1, -x_2)$, (y_1, y_2) (resp. (x_1, x_2) , $(y_1, -y_2)$), which gives a bigger (or equal) value for I . Hence, we can restrict our study to the case $x_2 \geq 0$ and $y_2 \leq 0$. We denote in spherical coordinates $x = (1, \theta)$, $y = (1, \eta)$, $z = (\|z\|, \gamma)$ and $w = (\|z\|, 2\pi - \gamma)$. Since $x, y \in \partial\mathcal{B}_1$, $x_1 \geq 0$, $y_1 \geq 0$, $x_2 \geq 0$

and $y_2 \leq 0$ then $\theta \in [0, \pi/2]$ and $\eta \in [3\pi/2, 2\pi]$. Furthermore, since $z, w \in \mathcal{B}_2$, we can easily verify that

$$\gamma \in [0, \pi/4), \quad (70)$$

since the straight line parallel to $e_1 + e_2$ does not intersect \mathcal{B}_2 , for every $\Delta \geq 2$.

With this notation we have

$$I(\theta, \eta) = \frac{1}{2}\|z\| \cos(\theta - \gamma) + \frac{1}{2}\|z\| \cos(\eta + \gamma) - \cos(\eta - \theta).$$

It then follows that the critical points of the above function have to satisfy

$$\frac{1}{2}\|z\| \sin(\theta - \gamma) + \sin(\eta - \theta) = 0, \quad \text{and} \quad -\frac{1}{2}\|z\| \sin(\eta + \gamma) + \sin(\eta - \theta) = 0.$$

Subtracting the two equations, since $\|z\| > 0$, we deduce that

$$\sin(\theta - \gamma) = -\sin(\eta + \gamma). \quad (71)$$

We observe that $\theta - \gamma \in [-\pi/2, \pi/2]$ and $\eta + \gamma \in [3\pi/2, 5\pi/2]$. Since $\sin(s)$ is injective for $s \in [-\pi/2, \pi/2]$, we deduce that the only solution is $\theta = 2\pi - \eta$. This critical point corresponds to a symmetric couple $x_1 = y_1, x_2 = -y_2$ and by Step 5 we have $I(x, y) \leq H(e_1, -e_1)$. Up to rotation, the boundary cases of θ and η coincide. Hence, we are just left to study the boundary case $\theta = 0$, or equivalently $(x, y) = (e_1, y)$ (the boundary case $\theta = \pi/2$ gives $x_1 \leq 0$ and will be treated in Step 7). In this case, since $y_1 \geq 0$ and $y_1, y_2, z_2 \in [-1, 1]$

$$I(e_1, y) = \frac{1}{2}z_1 + \frac{1}{2}y_1z_1 - \frac{1}{2}y_2z_2 - y_1 \leq \frac{1}{2}z_1(1 + y_1) + 1/2 < z_1 + 1 = H(e_1, -e_1).$$

Step 7. We solve Problem (69).

Proof of Step 7. We now assume that $x, y \in \partial\mathcal{B}_1$, $x_1 \leq 0, y_1 \geq 0$, $x^T z \geq y^T z$ and $y^T w \geq x^T w$. As explained in Step 6, we can also assume that $x_2 \geq 0$ and $y_2 \leq 0$. This implies that, using the notation of Step 6, we need to study the domain

$$(\theta, \eta) \in [\pi/2, \pi/2 + 2\gamma] \times [3\pi/2, 2\pi]. \quad (72)$$

Using a similar line of argument as in Step 6, all critical points in this region must satisfy (71). By (70), since the function $\sin(s)$ is strictly increasing in $[-\gamma, \pi/2 - \gamma]$ and $\sin(s) > \sin(\pi/2 - \gamma) = \sin(\pi/2 + \gamma)$ for every $s \in (\pi/2 - \gamma, \pi/2 + \gamma)$, it follows that $\sin([\pi/2 - \gamma, \pi/2 + \gamma]) \cap \sin([-\gamma, \pi/2 - \gamma]) = \{\sin(\pi/2 - \gamma)\}$ and that the equation (71) is never satisfied in the interior of the region (72). This implies that the only maximum points can be achieved at the boundary. We are just left to check that for all the boundary points (x, y) of this region, $I(x, y) \leq H(e_1, -e_1)$.

We start with $\theta = \pi/2$, that is, all the points of the form (e_2, y) with $y \in \partial\mathcal{B}_1$. We claim that

$$I(e_2, y) = \frac{1}{2}z_2 + \frac{1}{2}y_1z_1 - \frac{1}{2}y_2z_2 - y_2 \leq z_1 + 1, \quad \forall y \in \partial\mathcal{B}_1.$$

The maximum of the linear function $I(e_2, y)$ over $y \in \partial\mathcal{B}_1$ is attained at

$$\tilde{y} = \frac{(z_1, -(z_2 + 2))}{\sqrt{z_1^2 + (z_2 + 2)^2}}.$$

Hence, it suffices to show that the following inequality is valid:

$$I(e_2, \tilde{y}) = \frac{1}{2}z_2 + \frac{1}{2}\sqrt{z_1^2 + (z_2 + 2)^2} \leq z_1 + 1, \quad \Delta - 1 \leq z_1 \leq \Delta + 1, \quad 0 \leq z_2 \leq 1,$$

Defining $u = z_1 - \Delta$, the above inequality can be equivalently written as:

$$\sqrt{1 - u^2} \leq (u + \Delta) - \frac{(u + \Delta)^2}{4(u + \Delta + 2)}, \quad -1 \leq u \leq 1, \quad (73)$$

First, notice that the right hand side of inequality (73) is increasing in Δ , hence it suffices to show its validity at $\Delta = 2$. Second this expression is concave and hence can be lower bounded by its secant line, denoted by $au + b$; therefore, it suffices to show that $\sqrt{1 - u^2} \leq au + b$. Squaring both sides, we need to show that $(au + b)^2 + u^2 \geq 1$ for $-1 \leq u \leq 1$ and it can be checked that the latter inequality is valid.

The calculations for the boundary case $\eta = 3\pi/2$, that is all the points $(x, -e_2)$ with $x \in \partial\mathcal{B}_1$, are symmetric to the case $\theta = \pi/2$ (up to a rotation).

We now consider the boundary case $\eta = 2\pi$, that is all the points (x, e_1) with $x \in \partial\mathcal{B}_1$ and we claim that $I(x, e_1) \leq z_1 + 1$ for every $x \in \partial\mathcal{B}_1$. Indeed, since $z_1 \geq 1$

$$I(x, e_1) = \frac{1}{2}x_1z_1 + \frac{1}{2}x_2z_2 + \frac{1}{2}z_1 - x_1 = \left(\frac{1}{2} - \frac{1}{z_1}\right)x_1z_1 + \frac{1}{2}x_2z_2 + \frac{1}{2}z_1, \quad \forall x \in \partial\mathcal{B}_1.$$

Since $\frac{1}{z_1} \in (0, 1]$, we have $\left(\frac{1}{2} - \frac{1}{z_1}\right)x_1z_1 \leq \frac{1}{2}z_1$ and since $x_2, z_2 \in [-1, 1]$, we have

$$I(x, e_1) \leq \frac{1}{2}z_1 + \frac{1}{2}x_2z_2 + \frac{1}{2}z_1 \leq z_1 + 1 = H(e_1, -e_1), \quad \forall x \in \partial\mathcal{B}_1.$$

The last boundary case is $\theta = \pi/2 + 2\gamma$, for every $\eta \in [3\pi/2, 2\pi]$. In this case, we observe that $\theta - \gamma \geq 2\pi - \eta + \gamma$, where $\theta - \gamma$ is the angle between x and z and $2\pi - \eta + \gamma$ is the angle between y and z . Hence $x^T z \leq y^T z$ and

$$I(x, y) \leq \frac{1}{2}y^T z + \frac{1}{2}y^T w - x^T y \leq y_1z_1 + 1 \leq z_1 + 1 = H(e_1, -e_1).$$

This concludes the proof of Step 7. □

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