On the Hardness of K-Subspaces

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Abstract

In this report, we study the hardness and the approximability of the K-subspace problem. The K-subspace problem is an optimization problem. It takes as input a set of N data points in $\mathbb{R}^D$ and K positive integers $r_1, \ldots, r_K$, and outputs K subspaces represented by K matrices $U_1, \ldots, U_K$ each of which satisfies $U_k \in \mathbb{R}^{D \times r_k}$ and $U_k^\top U_k = I$ such that, when clustering those N data according to the nearest subspace, the sum of the squared distances between data and their nearest subspaces is minimized. Firstly, we prove that, even for $K = 2$ and $r_1 = \cdots = r_K$, it is NP-complete to decide if there exists K subspaces that contains all the data, i.e., the K-subspace objective is 0. This implies that it is NP-hard to approximate the K-subspaces problem to within factor α, for any finite $\alpha > 0$. Secondly, we prove that if $r := r_1 = \cdots = r_K$ is a fixed constant, the K-subspaces problem is APX-hard: there exists $\varepsilon > 0$ such that it is NP-hard to approximate the K-subspaces problem to within factor $(1 + \varepsilon)$.

1 Problem Formulation

Given a dataset $\mathcal{X} = \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^D$ of N data points in $\mathbb{R}^D$ which lie near the union of K unknown subspaces $\mathcal{S}_1, \ldots, \mathcal{S}_K$ with orthonormal bases $U_1, \ldots, U_K$ and dimensions $r_1, \ldots, r_K$, respectively. The goal of subspace clustering is to cluster the data points according to nearest subspace, which we now define formally.

Definition 1. The *K-Subspaces* (KSS) problem is an optimization problem which takes as input a data set $\mathcal{X} = \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^D$ and K positive integers $r_1, \ldots, r_K$, and outputs a partition $\mathcal{C} = \{C_1, \ldots, C_K\}$ of $\mathcal{X}$ and a collection of K matrices $\mathcal{U} = \{U_1, \ldots, U_K \mid U_k \in \mathbb{R}^{D \times r_k}, U_k^\top U_k = I\}$ such that the objective

$$\sum_{k=1}^{K} \sum_{x \in C_k} \left\| x - U_k U_k^\top x \right\|_2^2 \tag{1}$$

is minimized.

We present a family of inapproximability results. Firstly, we show that even for $K = 2$ and any finite $\alpha > 0$ which may depend on D, N, r, approximating the KSS objective to within factor α is NP-hard. Secondly, we show that the K-Subspaces is APX-hard for every fixed r. Notice that both hardness results are stronger than, and can be applied to the conventional NP-hardness result, where r, D, K and x_i's are inputs to the K-subspaces instance.

2 Inapproximability for $K = 2$

We will establish a reduction from the *balanced vertex separator* problem. Definition 2 and Theorem 3 below are on a special case of the results in [4, 2].

Definition 2. Given a graph $G = (V, E)$, a *balanced vertex separator* of size ℓ is a subset $S \subseteq V$ of vertices with $|S| = \ell$ such that $V \setminus S$ can be partitioned into two sets X_1, X_2 of equal size $|X_1| = |X_2|$ and for any $v_1 \in X_1, v_2 \in X_2$, $(v_1, v_2) \notin E$.

The proof of Theorem 7.1 in [2] can be used to prove the theorem below. We include the proof for completeness.

Theorem 3. *It is NP-complete to decide if a graph $G = (V, E)$ has a balanced vertex separator of size ℓ.*

Proof. It is easy to see that the problem is in NP, as (S, X_1, X_2) can be used as a yes certificate.

To show the problem is NP-hard, we reduce it from a well-known problem CLIQUE: given a graph $G = (V, E)$ and an integer k, decide if G has a clique of size k. Assume $u_1 \in V$ is known to belong to a clique of size k, if such clique exists. Such assumption can be made without loss of generality because there are at most n possible choices for u_1 and we can just try them all. We construct the balanced vertex separator instance $(\bar{G} = (\bar{V}, \bar{E}), \ell)$ as follows. Set $\ell = k$. $\bar{V}$ is defined as follows: create a vertex v_i in $\bar{V}$ for each $u_i \in V$; create a vertex v_{ij} in $\bar{V}$ for each $(u_i, u_j) \in E$; create a set of vertices $W \subseteq \bar{V}$ with $|W| = |V| + |E| - k^2$. $\bar{E}$ is defined as follows: create an edge $(v_i, v_j) \in \bar{E}$ for each $1 \leq i < j \leq |V|$ (i.e., the set V forms a clique in $\bar{G}$); include edges $(v_i, v_{ij}) \in \bar{E}$ and $(v_j, v_{ij}) \in \bar{E}$ for each $(u_i, u_j) \in E$; include $(w, v_1) \in \bar{E}$ for each $w \in W$.

If the CLIQUE instance is a yes instance and assume without loss of generality that $\{u_1, \ldots, u_k\}$ form a clique, it is straightforward to check that $S = \{v_1, \ldots, v_k\}$, $X_1 = W \cup \{v_{ij} : 1 \leq i < j \leq k\}$ and $X_2 = \bar{V} \setminus (S \cup X_1)$ give a valid vertex separator solution: all edges going out from X_1 are connected to S (in particular, none of them is connected to X_2), and $|X_1| = |X_2| = |V| + |E| - k - \binom{k}{2}$.

If the CLIQUE instance is a no instance, we aim to show that $\bar{G}$ does not have a balanced vertex separator of size $k = \ell$. Suppose otherwise a solution (S, X_1, X_2) exists. It must be that $|S| = k$ and $|X_1| = |X_2| = |V| + |E| - k - \binom{k}{2}$. Firstly, we must include

v_1 in S, for otherwise the connected component including v_1 after S's removal has size at least $|W| + |V| = 2|V| + |E| - k^2 > |V| + |E| - k - \binom{k}{2}$, which does not fit into any of X_1, X_2 (we can make sure $|V| \gg k$ in the CLIQUE instance by creating extra isolated vertices). Next, we try to fill vertices into X_1. We can put all vertices in W into X_1, as these vertices become isolated when v_1 is removed. We then still need to fill in another $(|V| + |E| - k - \binom{k}{2}) - (|V| + |E| - k^2) = \binom{k}{2}$ vertices into X_1. The only way to do this is to choose another $k - 1$ vertices from $v_2, \ldots, v_n$ for S such that the chosen k vertices correspond to a k-clique in G. However, this contradicts to that the CLIQUE instance is a no instance. □

Now we are ready to present our main result. The theorem below shows that it is NP-complete to decide if the minimum KSS objective value is 0, even for $K = 2$.

Theorem 4. *There exists r such that it is NP-complete to decide if there exists $\mathcal{C} = \{c_1, c_2\}$ and $\mathcal{U} = \{U_1, U_2\}$ such that*

$$\sum_{k=1}^{2} \sum_{i:x_i \in c_k} \left\| x_i - U_k U_k^\top x_i \right\|_2^2 = 0,$$

subjecting to $U_1, U_2 \in \mathbb{R}^{D \times r}$.

Proof. It is easy to see that the problem is in NP, as we can use $(\mathcal{C}, \mathcal{U})$ as a yes certificate.

To show the problem is NP-hard, we reduce it from the problem of finding a balanced vertex separator of size ℓ in a graph $G = (V, E)$, whose NP-completeness is established in Theorem 3. In this proof, let $e_i \in \mathbb{R}^{|V|}$ be the unit vector with the i-th coordinate being 1 and the remaining coordinates being 0. Given a vertex separator instance $(G = (V, E), \ell)$, we construct the following K-subspace instance:

- $r = \frac{1}{2}(|V| + \ell)$ (we assume $|V| + \ell$ is even; otherwise the balanced vertex separator instance is a trivial no instance);
- We create $N = |V| + 3|E|$ data in $\mathbb{R}^{|V|}$ as follows.
  - For each $v_i \in V$, create a datum $x_i = e_i$;
  - For each $(v_i, v_j) \in E$ (assume $i < j$), create three data $y_{ij}^0 = e_i + e_j$, $y_{ij}^1 = 0.5e_i + e_j$ and $y_{ij}^2 = e_i + 0.5e_j$.

To conclude the proof, we need to show the completeness and soundness:

1. If G has a balanced vertex separator of size ℓ, there exist $\mathcal{C}, \mathcal{U}$ such that the K-subspaces objective is 0.
2. If there exists $\mathcal{C}, \mathcal{U}$ such that the K-subspaces objective is 0, G has a balanced vertex separator of size ℓ.

To show 1, without loss of generality, let (S, X_1, X_2) be the balanced vertex separator solution with

$$X_1 = \left\{v_1, \dots, v_{\frac{|V|-\ell}{2}}\right\}, S = \left\{v_{\frac{|V|-\ell}{2}+1}, \dots, v_{\frac{|V|+\ell}{2}}\right\} \text{ and } X_2 = \left\{v_{\frac{|V|+\ell}{2}+1}, \dots, v_{|V|}\right\}.$$

We consider

$$U_1 = \begin{bmatrix} e_1 & e_2 & \cdots & e_{\frac{|V|+\ell}{2}} \end{bmatrix}, \qquad U_2 = \begin{bmatrix} e_{\frac{|V|-\ell}{2}+1} & e_{\frac{|V|-\ell}{2}+2} & \cdots & e_{|V|} \end{bmatrix},$$

and

$$c_1 = \left\{x_i : 1 \le i \le \frac{|V|+\ell}{2}\right\} \cup \left\{y_{ij}^0, y_{ij}^1, y_{ij}^2 : 1 \le i < j \le \frac{|V|+\ell}{2}\right\},$$
$$c_2 = \left\{x_i : \frac{|V|-\ell}{2} + 1 \le i \le |V|\right\} \cup \left\{y_{ij}^0, y_{ij}^1, y_{ij}^2 : \frac{|V|-\ell}{2} + 1 \le i < j \le |V|\right\}.$$

We can see that $c_1 \cup c_2$ covers all the N data: c_1 covers all those x_i's corresponding to vertices in $X_1 \cup S$, and all those y_{ij}^0's (or y_{ij}^1's, y_{ij}^2's) corresponding to edges in the subgraph induced by $X_1 \cup S$; c_2 covers all those x_i's corresponding to vertices in $S \cup X_2$, and all those y_{ij}^0's (or y_{ij}^1's, y_{ij}^2's) corresponding to edges in the subgraph induced by $S \cup X_2$. In particular, there is no such datum y_{ij}^0 (or y_{ij}^1, y_{ij}^2) corresponding to an edge between X_1, X_2, as S is a vertex separator. Moreover, by our construction, it is easy to see that any $x \in c_1$ is in the subspace spanned by all column vectors of U_1, implying that $\|x - U_1 U_1^\top x\|_2 = 0$. Similarly, for any $x \in c_2$, we have $\|x - U_2 U_2^\top x\|_2 = 0$. This implies that the K-subspaces objective is 0, concluding 1.

To show 2, suppose there exist $\mathcal{C}, \mathcal{U}$ such that the K-subspaces objective is 0. First of all, for each pair i, j with $(v_i, v_j) \in E$, we can assume without loss of generality that the three data $y_{ij}^0, y_{ij}^1, y_{ij}^2$ belong to the same cluster (either c_1 or c_2). In fact, $y_{ij}^0, y_{ij}^1, y_{ij}^2$ are linearly dependent. If any two of them are in the same subspace defined by either U_1 or U_2, the third one is also in this subspace. Thus, $y_{ij}^0, y_{ij}^1, y_{ij}^2$ are either in three different subspaces, or in a single subspace. Since we are only allow $K = 2$ subspaces, the K-subspaces objective being 0 implies that they are in a single subspace.

Let $V_1 \subseteq V$ be defined as

$$V_1 = \{v_i \in V : x_i \in c_1\} \cup \left\{v_i \in V : \exists j \text{ such that either } y_{ij}^0 \in c_1 \text{ or } y_{ji}^0 \in c_1\right\}.$$

In words, V_1 is the set of vertices v_i such that either the datum corresponding to v_i is in c_1 or the datum corresponding to an edge incident to v_i is contained in c_1. Similarly, define $V_2 \subseteq V$ as

$$V_2 = \{v_i \in V : x_i \in c_2\} \cup \left\{v_i \in V : \exists j \text{ such that either } y_{ij}^0 \in c_2 \text{ or } y_{ji}^0 \in c_2\right\}.$$

We will show that the subspace defined by U_1 has dimension at least $|V_1|$. To see this, consider the matrix $M_1 \in \mathbb{R}^{|V| \times |c_1|}$ whose columns are those data from c_1. By our construction, M_1 has exactly $|V_1|$ rows that are not all-zero. We claim that these $|V_1|$ rows are linearly independent. Suppose this is not true and there exists coefficients $a_1, \ldots, a_{|V_1|}$ such that the weighted sum of these $|V_1|$ rows is the zero vector and at least one of $a_1, \ldots, a_{|V_1|}$ is nonzero. Suppose $a_1 \neq 0$ and the i-th row of M_1 corresponds to a_1. Consider an arbitrary nonzero entry in the i-th row. The column containing this entry either corresponds to the datum x_i or one of $y_{ij}^0, y_{ij}^1, y_{ij}^2$. In the former case, this entry is the only nonzero entry this column, and assigning $a_1 \neq 0$ to row i cannot make the weighted sum of those $|V_1|$ rows a zero vector, which is a contradiction. In the latter case, the $|V| \times 3$ submatrix defined by the three columns representing $y_{ij}^0, y_{ij}^1, y_{ij}^2$ (M_1 contains all these three columns, because $y_{ij}^0, y_{ij}^1, y_{ij}^2$ belongs to the same cluster as we have shown earlier) is

$$\begin{bmatrix} 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ 1 & 0.5 & 1 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \\ 1 & 1 & 0.5 \\ 0 & 0 & 0 \\ \vdots & \vdots & \vdots \\ 0 & 0 & 0 \end{bmatrix},$$

where row i and j are the only two rows that are not all zero. If $a_1 \neq 0$ is assigned to row i, it is impossible to assign a coefficient to row j such that the weighted sum of the two rows is a zero vector. This again is a contradiction. Therefore, the $|V_1|$ nonzero rows in M_1 are linearly independent, so the rank of M_1 is $|V_1|$. Viewing this rank as column rank, this implies that the subspace containing all the data in c_1 has dimension at least $|V_1|$, so U_1 has dimension at least $|V_1|$. Thus, $|V_1| \leq \dim(U_1) = r = \frac{1}{2}(|V|+\ell)$. Similarly, $|V_2| \leq \frac{1}{2}(|V|+\ell)$. We arbitrarily add extra vertices in V_1, V_2 such that $|V_1| = |V_2| = \frac{1}{2}(|V| + \ell)$.

Since $c_1 \cup c_2$ contains all the data including $x_1, \ldots, x_{|V|}$, we have $V_1 \cup V_2 = V$. By inclusion-exclusion principle, $|V_1 \cap V_2| = \frac{1}{2}(|V| + \ell) + \frac{1}{2}(|V| + \ell) - |V| = \ell$. We claim that $S = V_1 \cap V_2$, $X_1 = V_1 \setminus V_2$ and $X_2 = V_2 \setminus V_1$ give a valid solution to the balanced vertex separator instance. It suffices to show that $(v_1, v_2) \notin E$ for any $v_1 \in X_1 = V_1 \setminus V_2$ and $v_2 \in X_2 = V_2 \setminus V_1$. Suppose this is not the case and $(v_1, v_2) \in E$. There is a datum y_{12}^0 and it must be contained in either c_1 or c_2. Assume without loss of generality that $y_{12}^0 \in c_1$. By our construction, both endpoints v_1, v_2 should be contained in V_1, which contradicts to $v_2 \in V_2 \setminus V_1$. We conclude 2 here. □

Theorem 4 straightforwardly implies the following corollary, which shows that the K-subspaces problem is totally inapproximable.

Corollary 5. *For any finite $\alpha > 0$ which may depend on D, N, K, r, approximating the K-subspaces objective function to within factor α is NP-hard, even for $K = 2$.*

3 Inapproximability for Fixed r

3.1 Inapproximability Result for $r = 1$

We first prove the following lemma.

Lemma 6. *Let t, r be two positive real numbers with $t > r$. Let $x \in \mathbb{R}^d$ with $\|x\|_2 \leq r$ and $y = (x, t)^\top \in \mathbb{R}^{d+1}$, and $\mathcal{S} = \{(x_1, \ldots, x_d, x_{d+1}) \in \mathbb{R}^{d+1} : x_{d+1} = t, \sum_{i=1}^d x_i^2 \leq r^2\}$ be the d-dimensional hyper-ball in the affine plane $\mathcal{A} = \{(x_1, \ldots, x_d, x_{d+1}) \in \mathbb{R}^{d+1} : x_{d+1} = t\}$, with center $p = (0, \ldots, 0, t)$ and radius r. Let $\mu = (\mu_1, \ldots, \mu_{d+1}) \in \mathbb{R}^{d+1}$ be a unit vector. Let $\nu = \frac{t}{\mu_{d+1}}(\mu_1, \ldots, \mu_d) \in \mathbb{R}^d$. We have*

$$\|y - \mu\mu^\top y\|_2 \leq \|x - \nu\|_2.$$

If in addition the line containing μ intersects $\mathcal{S}$, we also have

$$\|x - \nu\|_2 \leq \frac{t^2 + r^2}{t^2 - r^2}\|y - \mu\mu^\top y\|_2. \tag{2}$$

Proof. Firstly, it is straightforward to show that $\|x - \nu\|_2 = \|y - \frac{t}{\mu_{d+1}}\mu\|_2$.

Next, elementary calculus shows that $\xi = \mu^\top y$ is the minimizer for the function $f(\xi) := \|y - \xi\mu\|_2^2$, so we have $\|y - \mu\mu^\top y\|_2 \leq \|y - \frac{t}{\mu_{d+1}}\mu\|_2$, implying the first inequality in the lemma.

For the inequality in Eq. (2), let $u = \frac{t}{\mu_{d+1}}\mu$. We need to show that

$$\frac{\|y - \mu\mu^\top y\|_2}{\|x - \nu\|_2} = \frac{\|y - \mu\mu^\top y\|_2}{\|y - u\|_2} \geq \frac{t^2 - r^2}{t^2 + r^2}.$$

The vector $\mu\mu^\top y$ is the projection of y onto the subspace spanned by u. Also let $\mathcal{H} = \{x : x = u + \alpha(y - u), \alpha \in \mathbb{R}\}$ (in words, $\mathcal{H}$ is the affine line passing through both y and u), and let q be the projection of the zero vector $\underline{0}$ onto $\mathcal{H}$. Note that q, y, u are colinear, as are $u, \mu\mu^\top y, \underline{0}$. See Fig. 1 for an illustration. We have

$$\frac{\|y - \mu\mu^\top y\|_2}{\|y - u\|_2} = \frac{\|q\|_2}{\|u\|_2} = \frac{q^\top u}{\|q\|_2\|u\|_2}\ , \tag{3}$$

where the first equality is based on that the two right triangles in Fig. 1 sharing the vertex u are similar, and the second equality is by the definition of projection (the projection of u onto the line passing through $\underline{0}$ and q is exactly q, so $q^\top u = u^\top q = \|q\|_2 \cdot \|q\|_2$).

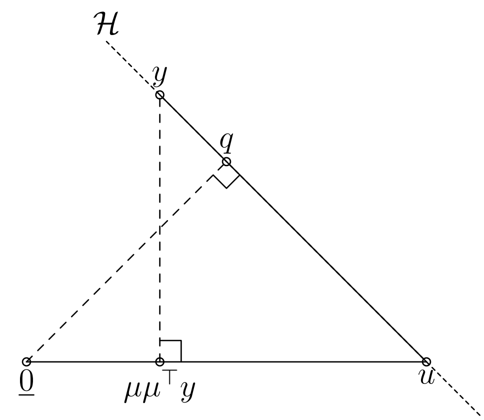

Figure 1: Illustration for Eq. (3).

Next, we will now show that $q, y, u \in \mathcal{S}$. By our assumption that the line containing μ intersects $\mathcal{S}$ and u is precisely this intersection, we have $u \in \mathcal{S}$. Since p is the center of $\mathcal{S}$ and $\|y - p\|_2 = \|x\|_2 \leq r$, we also have $y \in \mathcal{S}$. To show $q \in \mathcal{S}$, we show that q is the projection of p (the center of $\mathcal{S}$) onto $\mathcal{H}$. Suppose otherwise that $\hat{q} \in \mathcal{H}$ is the projection of p onto $\mathcal{H}$ and $\hat{q} \neq q$, then $\|p - \hat{q}\|_2 < \|p - q\|_2$. Since for all $a \in \mathcal{A}$, $(a - p)^\top p = 0$, and $q, \hat{q} \in \mathcal{H} \subseteq \mathcal{A}$, we have that

$$\begin{aligned} \|\underline{0} - \hat{q}\|_2^2 &= \|\underline{0} - p\|_2^2 + \|p - \hat{q}\|_2^2 && \text{(Pythagorean theorem)} \\ &< \|\underline{0} - p\|_2^2 + \|p - q\|_2^2 \\ &= \|\underline{0} - q\|_2^2, && \text{(Pythagorean theorem)} \end{aligned}$$

giving us a contradiction since q, instead of $\hat{q}$, was defined as the projection of $\underline{0}$ onto $\mathcal{H}$. Thus, q is the projection of p onto $\mathcal{H}$, implying $\|p - q\|_2 \leq \|p - w\|_2$ for all $w \in \mathcal{H}$, including $w = y$. Therefore, $\|p - q\|_2 \leq \|p - y\|_2 = \|x\|_2 \leq r$, implying $q \in \mathcal{S}$.

Finally, we will bound $q^\top u / \|q\|_2 \|u\|_2$ on the right hand side of Eq. (3). Since $q, u \in \mathcal{S}$ we have by the Pythagorean theorem that $\|q\|_2^2 \leq \|p\|_2^2 + r^2 = t^2 + r^2$ and similarly $\|u\|_2^2 \leq t^2 + r^2$. Thus, we have the following bound for the denominator.

$$\|q\|_2 \|u\|_2 \leq \sqrt{t^2 + r^2} \cdot \sqrt{t^2 + r^2} = t^2 + r^2.$$

For the numerator, we note that

$$q^\top u = t^2 + \sum_{i=1}^{d} q_i u_i \geq t^2 - \frac{1}{2} \left(\sum_{i=1}^{d} q_i^2 + \sum_{i=1}^{d} u_i^2 \right) \geq t^2 - r^2 ,$$

where the second last inequality is based on the inequality $ab \geq -\frac{1}{2}(a^2 + b^2)$ and the last inequality is based on that $q, u \in \mathcal{S}$.

Putting these together, we have

$$\frac{q^\top u}{\|q\|_2 \|u\|_2} \geq \frac{t^2 - r^2}{t^2 + r^2}. \tag{4}$$

Eq. (3) and Eq. (4) complete the proof. □

Now we are ready to present our hardness result. The theorem below shows that the K-subspace problem is APX-hard even for $r = 1$.

Theorem 7. *For $r = 1$, there exists $\varepsilon > 0$ such that it is NP-hard to approximate the optimal KSS objective*

$$\min_{\mathcal{C},\mathcal{U}} \sum_{k=1}^{K} \sum_{i:x_i \in c_k} \left\| x_i - U_k U_k^\top x_i \right\|_2^2$$

to within a factor of $(1+\varepsilon)$, subjecting to $U_k \in \mathbb{R}^{D\times r}$ for each $k = 1, \ldots, K$.

Proof. We will prove the lemma by a reduction from the Euclidean K-means problem. In [1], it has been shown that *there exists a constant $\epsilon > 0$ such that it is NP-hard to approximate the K-means objective to within a factor of $(1+\epsilon)$.*

Given a K-means instance $(\{\bar{x}_1, \ldots, \bar{x}_N : \bar{x}_i \in \mathbb{R}^{\bar{D}}\}, \bar{K})$, we construct the following KSS instance:

$$\big(\{x_1, \ldots, x_N : x_i \in \mathbb{R}^D\}, K\big) \quad \text{with} \quad \begin{array}{l} K = \bar{K}, D = \bar{D} + 1, \text{ and} \\ x_i = \begin{bmatrix} \bar{x}_i \\ T \end{bmatrix} \text{ for each } i = 1, \ldots, N, \end{array}$$

where $T > 0$ is a very large real number such that $(\frac{T^2 - 9d^2}{T^2 + 9d^2})^2 (1+\epsilon) - 1 > 0$ with $d = \max_i \|\bar{x}_i\|_2$. To prove the lemma, set

$$\varepsilon = \left(\frac{T^2 - 9d^2}{T^2 + 9d^2}\right)^2 (1+\epsilon) - 1,$$

and we aim to show that a $(1+\varepsilon)$-approximation algorithm for the above KSS instance will give a $(1+\epsilon)$-approximation to the optimal objective value of the K-means instance.

For any solution $(\mathcal{C} = \{c_1, \ldots, c_K\}, \mathcal{U} = \{U_1, \ldots, U_K\})$ to the KSS instance, let

$$\phi_{KSS}(\mathcal{C},\mathcal{U}) = \sum_{k=1}^{K} \sum_{i:x_i \in c_k} \left\| x_i - U_k U_k^\top x_i \right\|_2^2$$

be the corresponding KSS objective value. Similarly, for any solution $(\mathcal{C} = \{c_1, \ldots, c_K\}, S = \{s_1, \ldots, s_K\})$ to the K-means instance where $s_1, \ldots, s_K$ are the K centers, let

$$\phi_{KM}(\mathcal{C}, S) = \sum_{k=1}^{K} \sum_{i:\bar{x}_i \in c_k} \|\bar{x}_i - s_k\|_2^2$$

be the corresponding K-means objective value. Let $(\mathcal{C}^* = \{c_1^*, \dots, c_K^*\}, \mathcal{U}^* = \{U_1^*, \dots, U_K^*\})$ be the optimal solution to the KSS instance and $(\mathcal{C}^\dagger = \{c_1^\dagger, \dots, c_K^\dagger\}, S^\dagger = \{s_1^\dagger, \dots, s_K^\dagger\})$ be the optimal solution to the K-means instance.

Suppose we have the said $(1+\varepsilon)$-approximation algorithm for KSS, and obtain the approximately optimal solution $(\mathcal{C} = \{c_1, \dots, c_K\}, \mathcal{U} = \{U_1, \dots, U_K\})$ to the KSS instance:

$$\phi_{KSS}(\mathcal{C},\mathcal{U}) \leq (1+\varepsilon)\phi_{KSS}(\mathcal{C}^*,\mathcal{U}^*). \tag{5}$$

For each $k = 1, \dots, K$, let

$$U_k = [u_{k1} \quad u_{k2} \quad \cdots \quad u_{k\bar{D}} \quad u_{kD}]^\top,$$

and construct

$$s_k = \frac{T}{u_{kD}} \cdot [u_{k1} \quad u_{k2} \quad \cdots \quad u_{k\bar{D}}]^\top.$$

We will show that the obtained K-means solution $(\mathcal{C} = \{c_1, \dots, c_K\}, S = \{s_1, \dots, s_K\})$ is a $(1+\epsilon)$-approximation:

$$\phi_{KM}(\mathcal{C}, S) \leq (1+\epsilon)\phi_{KM}(\mathcal{C}^\dagger, S^\dagger). \tag{6}$$

Before showing (6), we construct the following solution to the KSS instance based on the K-means optimal solution $(\mathcal{C}^\dagger, S^\dagger)$:

$$(\mathcal{C}^\dagger, \mathcal{U}' = \{U_1', \dots, U_K'\}),$$

where

- the constructed KSS solution has the same partition, and
- $U_k' = \dfrac{(s_k^\dagger, T)}{\|(s_k^\dagger, T)\|_2}$. That is, each center point $s_k^\dagger \in \mathbb{R}^{\bar{D}}$ is appended with an extra coordinate T, and the resultant D-dimensional vector is then normalized.

The remaining part of this proof aims to show (6), and we show it by showing the following three inequalities.

$$\phi_{KM}(\mathcal{C}, S) \leq \left(\frac{T^2 + 9d^2}{T^2 - 9d^2}\right)^2 \phi_{KSS}(\mathcal{C},\mathcal{U}) \tag{7}$$

$$\phi_{KSS}(\mathcal{C}^*,\mathcal{U}^*) \leq \phi_{KSS}(\mathcal{C}^\dagger,\mathcal{U}') \tag{8}$$

$$\phi_{KSS}(\mathcal{C}^\dagger,\mathcal{U}') \leq \phi_{KM}(\mathcal{C}^\dagger, S^\dagger) \tag{9}$$

Let $\mathcal{S} = \{(x_1, \dots, x_D) \in \mathbb{R}^D : x_D = T, \sum_{i=1}^{\bar{D}} x_i \leq (3d)^2\}$ be the $\bar{D}$-dimensional ball in the affine plane $\{(x_1, \dots, x_D) \in \mathbb{R}^D : x_D = T\}$ with center $(0, \dots, 0, T)$ and radius $3d$. By our definition of d, all the data x_i's are within the ball with center $(0,\ldots,0,T)$ and radius d. Loosely speaking, we can assume without loss of generality that the line containing each U_k intersects $\mathcal{S}$: if any U_k misses $\mathcal{S}$, it is too far away from all the data x_i's, and straightforward geometric arguments can show that it is even better to replace U_k by the vector $(0,\ldots,0,1)$ that pointing towards the center of $\mathcal{S}$; thus, upon receiving the output $(\mathcal{C},\mathcal{U})$ of the mentioned $(1+\varepsilon)$-approximation algorithm, we can assume there is an extra cleanup step which replaces any U_k that misses $\mathcal{S}$ by $(0,\ldots,0,1)$.

By the second inequality in Lemma 6,

$$\phi_{KM}(\mathcal{C},S)=\sum_{k=1}^{K}\sum_{i:\bar{x}_i\in c_k}\|\bar{x}_i-s_k\|_2^2\le\sum_{k=1}^{K}\sum_{i:x_i\in c_k}\left(\frac{T^2+9d^2}{T^2-9d^2}\right)^2\left\|x_i-U_kU_k^\top x_i\right\|_2^2$$
$$=\left(\frac{T^2+9d^2}{T^2-9d^2}\right)^2\phi_{KSS}(\mathcal{C},\mathcal{U}),$$

which concludes Eq. (7).

Since $(\mathcal{C}^*,\mathcal{U}^*)$ is the optimal solution to the KSS instance while $(\mathcal{C}^\dagger,\mathcal{U}')$ may not be optimal, (8) holds. A straightforward application of the first inequality of Lemma 6 can also show (9).

Finally, applying inequalities (7), (5), (8) and (9) one-by-one, and by our definition of ε, we obtain Eq. (6). □

3.2 Inapproximability Result for General Fixed r

In this section, we prove the following theorem.

Theorem 8. *For any fixed constant r, there exists $\varepsilon>0$ such that it is NP-hard to approximate the optimal KSS objective*

$$\min_{\mathcal{C},\mathcal{U}}\sum_{k=1}^{K}\sum_{i:x_i\in c_k}\left\|x_i-U_kU_k^\top x_i\right\|_2^2$$

to within a factor of $(1+\varepsilon)$, subjecting to $U_k\in\mathbb{R}^{D\times r}$ for each $k=1,\ldots,K$.

Since the theorem for $r=1$ has been proved in the last section, we consider $r\ge 2$ in this section.

The construction Given a K-means instance $(\{\bar{x}_1,\ldots,\bar{x}_{\bar{N}}:\bar{x}_i\in\mathbb{R}^{\bar{D}}\},\bar{K})$, we construct the KSS instance as follows.

- $K=\bar{K}$ and $D=\bar{D}+r$;

- For each $\bar{x}_n$ in the K-means instance, construct M^{r-1} data for the KSS instance

$$X_n = \{x_n^{i_1,\dots,i_{r-1}} : i_1, \dots, i_{r-1} \in \{0, 1, \dots, M-1\}\}$$

  such that

$$x_n^{i_1,\dots,i_{r-1}} = [\bar{x}_n \quad T \quad i_1 \cdot S \quad \cdots \quad i_{r-1} \cdot S]^\top \in \mathbb{R}^D,$$

  where $T, S > 0$ are two large real numbers and $M \in \mathbb{Z}^+$ is a large integer to be defined later.

Notice that the total number of data in the constructed KSS instance is $N = M^{r-1} \cdot \bar{N}$.

Let $d = \max_{i \in \{1,\dots,\bar{N}\}} \|\bar{x}_i\|$. For each $i_1, \dots, i_{r-1}$, let

$$\mathcal{S}^{i_1,\dots,i_{r-1}} = \left\{ x = (x_1, \dots, x_D) \in \mathbb{R}^D : x_{\bar{D}+1} = T, x_{\bar{D}+2} = i_1 S, \dots, x_{\bar{D}+r} = i_{r-1} S, \sum_{i=1}^{\bar{D}} x_i \le d^2 \right\}$$

be the hyper-ball in the affine hyper-plane

$$\left\{ x = (x_1, \dots, x_D) \in \mathbb{R}^D : x_{\bar{D}+1} = T, x_{\bar{D}+2} = i_1 S, \dots, x_{\bar{D}+r} = i_{r-1} S \right\}$$

centered at $(0, \dots, 0, T, i_1 S, \dots, i_{r-1} S)$ with radius d. Although we will define T, S, M later, it is helpful to first notice that we will make $S \gg 2d$ so that all those hyper-balls are far away from each other. Let

$$\mathcal{B} = \left\{ x = (x_1, \dots, x_D) \in \mathbb{R}^D : x_{\bar{D}+1} = T, \sum_{i \neq \bar{D}+1} x_i^2 \le (\sqrt{r} M S + d)^2 \right\}$$

be the hyper-ball that is large enough to contain all the data points in our KSS instance. We will, in addition, make T significantly larger than the radius $\sqrt{r} M S + d$ of $\mathcal{B}$, such that the line passing through the origin and an arbitrary point in $\mathcal{B}$ has very small angle to the $(\bar{D}+1)$-th unit vector.

The high level ideas of the proof The K-means instance is duplicated M^{r-1} times such that each $\mathcal{S}^{i_1,\dots,i_{r-1}}$ contains a copy of the instance. Moreover, the centers of the hyper-balls $\{\mathcal{S}^{i_1,\dots,i_{r-1}}\}$ form a lattice structure with spacing S, and the data corresponding to each K-means instance copy are very close (compared to the spacing S) to the respective center.

In an (approximately) optimal solution to the constructed KSS instance, each subspace U_k needs to intersect, or at least not far away from, all the M^{r-1} hyper-balls. Specifically, let e_i be the i-th unit vector in $\mathbb{R}^D$, the r columns of U_k need to be approximately $e_{\bar{D}+1}, \dots, e_{\bar{D}+r}$. Otherwise, if the $(j+1)$-th column has a large difference to $e_{\bar{D}+j+1}$, then, for any $i_1, \dots, i_{j-1}, i_{j+1}, \dots, i_{r-1}$, U_k will intersect very few hyper-balls from

$\{\mathcal{S}^{i_1,\dots,i_{r-1}} : r_j = 0, 1, \dots, M-1\}$. The total number of hyper-balls that U_k intersects is at most about $c \cdot M^{r-2} \ll M^{r-1}$ (for some $c \ll M$), and the cost for allocating those data in the not-intersected balls in the cluster C_k is high. Therefore, to avoid the high cost, the data in each ball that U_k does not intersect can only be allocated to one of the remaining $K-1$ subspaces that intersect (or is close to) the ball. As a result, although such U_k may do a better job for those data in the cM^{r-2} balls that it intersects, but it will leave the data in the remaining $M^{r-1} - cM^{r-2}$ balls to the remaining $K-1$ subspaces to cover. Since $M^{r-1} - cM^{r-2}$ is considerably larger than cM^{r-2}, switching U_k to some U'_k that intersects all the balls is much more beneficial.

Next, if each U_k intersects all the M^{r-1} balls, it is easy to see that the intersection between U_k and each ball can only be a single point: intuitively, if U_k spends more than 0 dimension to a ball, it will not have enough dimensions to cover all the balls whose centers form an $(r-1)$-dimensional lattice. By showing a lemma that is similar to Lemma 6, we can show that the distance between a data point and its closest subspace U_k is approximately the distance between it and the point at which U_k and the ball containing the data point intersect. For each ball $\mathcal{S}^{i_1,\dots,i_{r-1}}$, by viewing its K intersections to $U_1, \dots, U_K$ as the K centers in the K-means problem, we find an approximate solution to the K-means instance. If we have an ε-approximated optimal solution to the KSS instance, we have M^{r-1} solutions to the K-means instance. Taking the best solution from them gives us an approximated optimal solution to the K-means instance.

The proof Let d and $\mathcal{S}^{i_1,\dots,i_{r-1}}$ be as defined in the last part. Let

$$\mathcal{P}^{i_1,\dots,i_{r-1}} = \{(x_1, \dots, x_D) : x_{\bar{D}+1} = T, x_{\bar{D}+2} = i_1 S, \dots, x_D = i_{r-1} S\}$$

be the hyperplane that contains $\mathcal{S}^{i_1,\dots,i_{r-1}}$. We will prove Theorem 8 following the ideas in the last part.

Proposition 9. *If a subspace $U_k \in \mathbb{R}^{D\times r}$ intersects at least $M^{r-2}+1$ hyperplanes from $\{\mathcal{P}^{i_1,\dots,i_{r-1}} : i_1, \dots, i_{r-1} \in \{0, 1, \dots, M-1\}\}$, then the intersection between U_k and a hyperplane it intersects is a single point. In particular, if a subspace $U_k \in \mathbb{R}^{D\times r}$ intersects at least $M^{r-2}+1$ hyper-balls from $\{\mathcal{S}^{i_1,\dots,i_{r-1}} : i_1, \dots, i_{r-1} \in \{0, 1, \dots, M-1\}\}$, then the intersection between U_k and a hyper-ball it intersects is a single point.*

Proof. For the ease of notation, we index each hyperplane $\mathcal{P}^{i_1,\dots,i_{r-1}}$ by a single integer $j \in \{0, 1, \dots, M^{r-1}-1\}$:

$$\mathcal{P}_j := \mathcal{P}^{i_1,\dots,i_{r-1}} \qquad \text{where } j = \sum_{s=1}^{r-1} i_s \cdot M^{s-1}.$$

Suppose for the sake of contradiction that U_k intersects at least $M^{r-2}+1$ hyper-balls and there exists $\mathcal{P}_{j^*}$ such that U_k intersects it at at least two points: z_{j^*} and z'_{j^*}. For each j such that U_k intersects $\mathcal{P}_j$, let z_j be the intersection of U_k and $\mathcal{P}_j$ (or one of the intersection points if the intersection is more than a single point). For each z_j, let $z_j^- \in \mathbb{R}^r$ be the truncated vector which consists of the last r entries of z_j. That is, the first entry of z_j^- is T, and the remaining $r-1$ entries are the values of $i_1 S, \ldots, i_{r-1} S$. As a first step, we show that there exists $r-1$ indices $j_1, \ldots, j_{r-1}$ such that U_k intersects $\mathcal{P}_{j_1}, \ldots, \mathcal{P}_{j_{r-1}}$ at $z_{j_1}, \ldots, z_{j_{r-1}}$ and the r vectors $z_{j^*}^-, z_{j_1}^-, \ldots, z_{j_{r-1}}^-$ are linearly independent.

Suppose this is not the case, and we can find at most $r' \leq r-2$ indices $j_1, \ldots, j_{r'}$ satisfying this. For any j such that U_k intersects $\mathcal{P}_j$ at z_j, the corresponding z_j^- must be in the r'-dimensional subspace spanned by $z_{j^*}^-, z_{j_1}^-, \ldots, z_{j_{r'}}^-$. Let $Z = \{(z_1, \ldots, z_r) : z_1 = T; z_2, \ldots, z_r \in \{0, 1, \ldots, M-1\}\}$ be the set of all possible values of z_j^-. We will derive a contradiction by showing that the subspace spanned by $z_{j^*}^-, z_{j_1}^-, \ldots, z_{j_{r'}}^-$ overlaps to Z at at most $M^{r'}$ points (since $M^{r'} \leq M^{r-2}$, this contradicts to that U_k intersects at least $M^{r-2}+1$ hyper-balls). Since $z_{j^*}^-, z_{j_1}^-, \ldots, z_{j_{r'}}^-$ are linearly independent, we can find $t_1, \ldots, t_{r'+1}$ such that the $(r'+1) \times (r'+1)$ submatrix from the rank-$(r'+1)$ matrix $[z_{j^*}^- \quad z_{j_1}^- \quad \cdots \quad z_{j_{r'}}^-]$ obtained by taking rows $t_1, \ldots, t_{r'+1}$ is non-degenerated. Moreover, we choose $t_1 = 1$. Then, for each z_j^- that is given by a linear combination of $z_{j^*}^-, z_{j_1}^-, \ldots, z_{j_{r'}}^-$, once the t_1-th, ..., $t_{r'+1}$-th entries are determined, the remaining $r - r' - 1$ entries are also determined. Since the t_1-th entry, which is the first entry, is always T, the number of possible choices for the $r'+1$ entries, the t_1-th, ..., $t_{r'+1}$-th entries, are $M^{r'}$. This implies that there are at most $M^{r'}$ points from Z that are in the subspace spanned by $z_{j^*}^-, z_{j_1}^-, \ldots, z_{j_{r'}}^-$, which gives us the desired contradiction.

In the next step, we show that, if the subspace defined by U_k contains those $r+1$ vectors $z_{j^*}, z'_{j^*}, z_{j_1}, \ldots, z_{j_{r-1}}$, it must has dimension at least $r+1$, which leads to a contradiction. We show this by showing that those $r+1$ vectors are linearly independent. Notice that the last r entries of z_{j^*}, z'_{j^*} are identical. The first $\bar{D}$ entries of them should be different. Let $z_{j^*} = [x \quad z_{j^*}^-]^\top$ and $z'_{j^*} = [x' \quad z_{j^*}^-]^\top$, and we know $x \neq x'$.

Suppose $z_{j^*}, z'_{j^*}, z_{j_1}, \ldots, z_{j_{r-1}}$ are linearly dependent. There exists $c_{j^*}, c'_{j^*}, c_1, \ldots, c_{r-1}$ such that $c_{j^*} z_{j^*} + c'_{j^*} z'_{j^*} + c_1 z_{j_1} + \cdots + c_{r-1} z_{j_{r-1}} = 0$, where $c_{j^*}, c'_{j^*}, c_1, \ldots, c_{r-1}$ are $r+1$ real numbers such that at least one of them is nonzero. Since this equality implies $(c_{j^*} + c'_{j^*}) z_{j^*}^- + c_1 z_{j^*}^- + \cdots + c_{r-1} z_{j_{r-1}}^- = 0$ and $z_{j^*}^-, z_{j^*}^-, \ldots, z_{j_{r-1}}^-$ are linearly independent, we know that $c_{j^*} = -c'_{j^*}$ and $c_1 = \cdots = c_{r-1} = 0$. However, since $x \neq x'$, the first $\bar{D}$ entries of $c_{j^*} z_{j^*} + c'_{j^*} z'_{j^*} + c_1 z_{j_1} + \cdots + c_{r-1} z_{j_{r-1}}$ cannot be all 0's, which is a contradiction. This proves the first statement in the proposition.

The implication from the first statement to the second is straightforward, since intersecting $\mathcal{S}^{i_1, \ldots, i_{r-1}}$ implies intersecting $\mathcal{P}^{i_1, \ldots, i_{r-1}}$, and the intersection between U_k and $\mathcal{P}^{i_1, \ldots, i_{r-1}}$ being a single point implies that the intersection between U_k and $\mathcal{S}^{i_1, \ldots, i_{r-1}}$ can at most be a single point. $\square$

The proposition below shows that, when S and T are sufficiently large, if a subspace U_k intersects at least $M^{r-2}+1$ hyper-balls, then the i-th column of U_k is very close to the

$(\bar{D}+i)$-th unit vector, up to a change of orthonormal basis.

Proposition 10. *Suppose $S > r(2d+1)^3 + 2rMd^2$ and $T > S + 4rMd^2$. If a subspace $U \in \mathbb{R}^{D\times r}$ intersects at least $M^{r-2}+1$ hyper-balls from $\{\mathcal{S}^{i_1,\ldots,i_{r-1}} : i_1,\ldots,i_{r-1} \in \{0,1,\ldots,M-1\}\}$, then, up to a change of orthonormal basis, we have $U = [u_1 \quad \cdots u_r]$ where*

- *$u_1 = [\kappa_1 \quad \tau \quad 0 \quad \cdots \quad 0]$ where $\kappa_1 \in \mathbb{R}^{\bar{D}}$ satisfies $\|\kappa_1\| < \frac{rMd}{T}$ and $\tau > \sqrt{1-(\frac{rMd}{T})^2}$, and*
- *for each $i = 2,\ldots,r$, $u_i = [\kappa_i \quad \xi_{i0} \quad \xi_{i1} \quad \cdots \quad \xi_{i(i-2)} \quad \sigma \quad 0 \quad \cdots \quad 0]$ where $\kappa_i \in \mathbb{R}^{\bar{D}}$ satisfies $\|\kappa_i\| < \frac{2d+1}{S}$, $\xi_{i0} \in \mathbb{R}$ satisfies $|\xi_{i0}| < \frac{4rMd^2}{ST}$, each $\xi_{ij} \in \mathbb{R}$ (with $1 \le j \le i-2$) satisfies $|\xi_{ij}| < \frac{(2d+1)^2}{S^2}$, and $\sigma > \sqrt{1 - \frac{(2d+1)^2}{S^2} - \frac{16r^2M^2d^4}{S^2T^2} - \frac{(i-2)(2d+1)^4}{S^4}}$.*

Proof. The high level ideas of this proof is as follows: firstly, we find r linearly independent vectors $v_1,\ldots,v_r$ that U must contain; secondly, we show that we can orthonormalise those r vectors to $u_1,\ldots,u_r$ satisfying the requirements in the proposition. Since U is an r-dimensional subspace, and $UU^\top$ is invariant up to a change of orthonormal basis, these will implies our proposition.

To construct $v_1,\ldots,v_r$, we first show that *for each $j = 1,\ldots,r-1$, there exist r positive integers $i_1^{(j)},\ldots,i_{j-1}^{(j)},i_j,i_j',i_{j+1}^{(j)},\ldots,i_{r-1}^{(j)} \in \{0,1,\ldots,M-1\}$ with $i_j \ne i_j'$ such that U intersects both $\mathcal{S}^{i_1^{(j)},\ldots,i_{j-1}^{(j)},i_j,i_{j+1}^{(j)},\ldots,i_{r-1}^{(j)}}$ and $\mathcal{S}^{i_1^{(j)},\ldots,i_{j-1}^{(j)},i_j',i_{j+1}^{(j)},\ldots,i_{r-1}^{(j)}}$*. Intuitively, this claim says that you can find at least two hyper-balls along each of the $r-1$ directions that U intersects. This is easy to show straightforwardly. Suppose for certain j we cannot find two balls intersected by U that only differ in the j-th "coordinate" i_j. Then all the intersected balls must have different values for the remaining $r-2$ "coordinates": $i_1,\ldots,i_{j-1},i_{j+1},\ldots,i_{r-1}$. However, there can be at most M^{r-2} such balls, which contradicts to that U intersects at least $M^{r-2}+1$ balls.

With this claim, we are ready to construct $v_1,\ldots,v_r$. For each $j = 2,\ldots,r$, define v_j as follows. Find the two balls $\mathcal{S}^{i_1^{(j-1)},\ldots,i_{j-2}^{(j-1)},i_{j-1},i_j^{(j-1)},\ldots,i_{r-1}^{(j-1)}}$ and $\mathcal{S}^{i_1^{(j-1)},\ldots,i_{j-2}^{(j-1)},i_{j-1}',i_j^{(j-1)},\ldots,i_{r-1}^{(j-1)}}$ that U intersects. Then the two intersection points (notice that Proposition 9 makes sure each intersection is a point) must be

$$\left[\bar{x}_{j1} \quad T \quad i_1^{(j-1)}S \quad \cdots \quad i_{j-2}^{(j-1)}S \quad i_{j-1}S \quad i_j^{(j-1)}S \quad \cdots \quad i_{r-1}^{(j-1)}S\right]$$

and

$$\left[\bar{x}_{j2} \quad T \quad i_1^{(j-1)}S \quad \cdots \quad i_{j-2}^{(j-1)}S \quad i_{j-1}'S \quad i_j^{(j-1)}S \quad \cdots \quad i_{r-1}^{(j-1)}S\right]$$

for certain $\bar{x}_{j1}, \bar{x}_{j2} \in \mathbb{R}^{\bar{D}}$ with two norms bounded by d. Let v_j be the difference between this two intersection points divided by $(i_{j-1} - i_{j-1}')$ (which should also be contained in U):

$$v_j = [\bar{x}_j \quad 0 \quad 0 \quad \cdots \quad 0 \quad S \quad 0 \quad \cdots \quad 0],$$

where $\bar{x}_j := \frac{1}{i_{j-1}-i'_{j-1}}(\bar{x}_{j1} - \bar{x}_{j2}) \in \mathbb{R}^{\bar{D}}$ satisfies $\|\bar{x}_j\| \leq \frac{2d}{i_{j-1}-i'_{j-1}} \leq 2d$ by the triangle inequality. To construct v_1, we take an arbitrary ball $\mathcal{S}^{i_1^\dagger,\dots,i_{r-1}^\dagger}$ that U intersect. Let v'_1 be the point of intersection (or the vector pointing from the origin to the point of intersection). We have

$$v'_1 = \begin{bmatrix} \bar{x}^\dagger & T & i_1^\dagger \cdot S & \cdots & i_{r-1}^\dagger \cdot S \end{bmatrix}$$

for certain $x^\dagger \in \mathbb{R}^{\bar{D}}$ such that $\|\bar{x}^\dagger\| \leq d$. Let

$$v_1 = v'_1 - \sum_{j=2}^{r} i_{j-1}^\dagger \cdot v_j = [\bar{x}_1 \quad T \quad 0 \quad \cdots \quad 0],$$

where $\bar{x}_1 = \bar{x}^\dagger - \sum_{j=2}^r i_{j-1}^\dagger \cdot \bar{x}_j$. We have $\|\bar{x}_1\| \leq d + \sum_{j=2}^r i_{j-1}^\dagger \cdot d < rMd$. Moreover, since $v'_1, v_2, \dots, v_r$ belong to the subspace U, v_1, being a linear combination of those, also belongs to U.

Next, we transform $v_1, \dots, v_r$ to orthonormal $u_1, \dots, u_r$. Intuitively, when S and T are very large, $v_1, \dots, v_r$ are almost orthogonal such that $v_1 \approx Te_{\bar{D}+1}$ and $v_i \approx Se_{\bar{D}+i}$ for $i \geq 2$. After the Gram-Schmidt process, those r vectors are only changed by a little bit, and the $(\bar{D}+i)$-th coordinate of u_i is almost 1, which implies the proposition. The detailed calculations are as follows.

We will show that, after orthogonalization but before normalization, $u_1, \dots, u_r$ are as follows:

$$\begin{array}{rcl} u_1 &=& [x_1 \quad T \quad 0 \quad 0 \quad 0 \quad \cdots \quad 0] \\ u_2 &=& [x_2 \quad \xi_{20} \quad S \quad 0 \quad 0 \quad \cdots \quad 0] \\ u_3 &=& [x_3 \quad \xi_{30} \quad \xi_{31} \quad S \quad 0 \quad \cdots \quad 0] \\ u_4 &=& [x_4 \quad \xi_{40} \quad \xi_{41} \quad \xi_{42} \quad S \quad \cdots \quad 0] \\ && \vdots \\ u_r &=& [x_r \quad \xi_{r0} \quad \xi_{r1} \quad \xi_{r2} \quad \xi_{r3} \quad \cdots \quad S] \end{array}$$

where

- $x_1 \in \mathbb{R}^{\bar{D}}$ satisfies $\|x_1\| < rMd$,
- $x_i \in \mathbb{R}^{\bar{D}}$ for each $i \geq 2$ satisfies $\|x_i\| < 2d + 1$,
- $|\xi_{i0}| < \frac{4rMd^2}{T}$ for each $i = 2, \dots, r$, and
- $|\xi_{ij}| < \frac{(2d+1)^2}{S}$ for each $i = 2, \dots, r$ and each j with $1 \leq j \leq i - 2$.

This can be shown by induction. For the base step, we know $u_1 = v_1$, so $\|x_1\| = \|\bar{x}_1\| < rMd$. For u_2, since $u_2 = v_2 - \frac{v_2^\top u_1}{\|u_1\|^2} u_1$ in the Gram-Schmidt process, we have

$$\|x_2\| = \left\| \bar{x}_2 - \frac{\bar{x}_2^\top x_1}{\|x_1\|^2 + T^2} x_1 \right\| < \|\bar{x}_2\| + \frac{\|\bar{x}_2\| \|x_1\|^2}{T^2} \leq 2d + \frac{2d \times rMd}{T^2} < 2d + 1,$$

and

$$|\xi_{20}| = \left|0 - \frac{\bar{x}_2^\top x_1}{\|x_1\|^2 + T^2} T\right| < \frac{\|\bar{x}_2\|\|x_1\|}{T} \leq \frac{2d \times rMd}{T} < \frac{4rMd^2}{T}.$$

Since the remaining coordinates of u_1 are 0, the remaining coordinates of u_2 are identical to those of v_2. This concludes the base step.

For the inductive step, suppose our claim holds for $u_1, \dots, u_i$. We consider u_{i+1}. Firstly, we only need to check for x_{i+1} and $\xi_{(i+1)0}, \dots, \xi_{(i+1)(i-1)}$, as the remaining coordinates of u_{i+1} are identical to those in v_{i+1} since these coordinates for each of $u_1, \dots, u_i$ are 0 by the induction hypothesis. For x_{i+1}, we have

$$\begin{aligned}
\|x_{i+1}\| &= \left\|\bar{x}_{i+1} - \sum_{s=1}^{i} \frac{v_{i+1}^\top u_s}{\|u_s\|^2} x_s\right\| \\
&= \left\|\bar{x}_{i+1} - \sum_{s=1}^{i} \frac{\bar{x}_{i+1}^\top x_s}{\|x_s\|^2 + \xi_{s0}^2 + \dots + \xi_{s(s-2)}^2 + S^2} x_s\right\| \\
&< 2d + \sum_{s=1}^{i} \frac{2d\|x_s\|^2}{S^2} && \text{(since } \|\bar{x}_{i+1}\| \leq 2d\text{)} \\
&< 2d + \frac{2d \cdot rMd}{S^2} + \frac{2d}{S^2} \cdot (i-1)(2d+1)^2 && \text{(induction hypothesis)} \\
&< 2d + 1. && \text{(since } S^2 > S > r(2d+1)^3 + 2rMd^2\text{)}
\end{aligned}$$

For $\xi_{(i+1)0}$, we have

$$\begin{aligned}
\|\xi_{(i+1)0}\| &= \left\|0 - \frac{v_{i+1}^\top u_1}{\|u_1\|^2} T - \sum_{s=2}^{i} \frac{v_{i+1}^\top u_s}{\|u_s\|^2} \xi_{s0}\right\| \\
&= \left\|-\frac{\bar{x}_{i+1}^\top x_1}{\|x_1\|^2 + T^2} T - \sum_{s=2}^{i} \frac{\bar{x}_{i+1}^\top x_s}{\|x_s\|^2 + \xi_{s0}^2 + \dots + \xi_{s(s-2)}^2 + S^2} \xi_{s0}\right\| \\
&< \frac{2d\|x_1\|}{T} + \sum_{s=2}^{i} \frac{2d\|x_s\|}{S^2} |\xi_{s0}| && \text{(since } \|\bar{x}_{i+1}\| \leq 2d\text{)} \\
&< \frac{2rMd^2}{T} + \frac{r \cdot 2d(2d+1)}{S^2} \frac{4rMd^2}{T} && \text{(by induction hypothesis)} \\
&< \frac{2rMd^2}{T} + \frac{1}{S(2d+1)} \frac{4rMd^2}{T} && \text{(since } S > r(2d+1)^3\text{)} \\
&< \frac{2rMd^2}{T} + \frac{2rMd^2}{T} && \text{(obviously } S(2d+1) > 2\text{)} \\
&= \frac{4rMd^2}{T}.
\end{aligned}$$

For each $\xi_{(i+1)j}$ with $1 \le j \le i-1$, we have

$$
\begin{aligned}
&\|\xi_{(i+1)j}\| \\
=&\left\| 0 - \frac{v_{i+1}^\top u_{j+1}}{\|u_{j+1}\|^2} S - \sum_{s=j+2}^{i} \frac{v_{i+1}^\top u_s}{\|u_s\|^2} \xi_{sj} \right\| \qquad \text{(the last term vanishes if } i < j+2) \\
=&\left\| - \frac{\bar{x}_{i+1}^\top x_{j+1} \cdot S}{\|x_{j+1}\|^2 + \xi_{(j+1)0}^2 + \cdots + \xi_{(j+1)(j-1)}^2 + S^2} - \sum_{s=j+2}^{i} \frac{\bar{x}_{i+1}^\top x_s \cdot \xi_{sj}}{\|x_s\|^2 + \xi_{s0}^2 + \cdots + \xi_{s(s-2)}^2 + S^2} \right\| \\
<&\frac{2d(2d+1)}{S} + \frac{r \cdot 2d(2d+1)}{S^2} \frac{(2d+1)^2}{S} \\
<&\frac{2d(2d+1)}{S} + \frac{1}{r(2d+1)^4} \frac{(2d+1)^2}{S} \qquad \text{(since } S > r(2d+1)^3) \\
<&\frac{2d(2d+1)}{S} + \frac{1}{S} < \frac{(2d+1)^2}{S}.
\end{aligned}
$$

Finally, by normalizing $u_1, \dots, u_r$ to unit vectors, the proposition follows easily. □

Proposition 9 and Proposition 10 imply the following corollary.

Corollary 11. *Suppose $S > r(2d+1)^3 + 2rMd^2$ and $T > S + 4rMd^2$.. If a subspace $U \in \mathbb{R}^{D \times r}$ intersects at least $M^{r-2}+1$ hyper-balls from $\{\mathcal{S}^{i_1,\dots,i_{r-1}} : i_1, \dots, i_{r-1} \in \{0, 1, \dots, M-1\}\}$, then U intersects each hyperplane $\mathcal{P}^{i_1,\dots,i_{r-1}}$ at exactly one point.*

Proof. Proposition 10 shows that $U = [u_1 \quad \cdots \quad u_r]$, where $u_1, \dots, u_r$ are as defined in the statement of Proposition 10. A point in U can be represented as $x = c_1 u_1 + \cdots + c_r u_r$ for certain $c_1, \dots, c_r \in \mathbb{R}$. It is also in $\mathcal{P}^{i_1,\dots,i_{r-1}}$ if the last r coordinates of x are $T, i_1 S, \dots, i_{r-1} S$ respectively. Therefore, the intersection between U and $\mathcal{P}^{i_1,\dots,i_{r-1}}$ are exactly those $x = c_1 u_1 + \cdots + c_r u_r$ subjecting to

$$
c_1 \begin{bmatrix} \tau \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} \xi_{20} \\ \sigma \\ 0 \\ \vdots \\ 0 \end{bmatrix} + c_3 \begin{bmatrix} \xi_{30} \\ \xi_{31} \\ \sigma \\ \vdots \\ 0 \end{bmatrix} + \cdots + c_r \begin{bmatrix} \xi_{r0} \\ \xi_{r1} \\ \xi_{r2} \\ \vdots \\ \sigma \end{bmatrix} = \begin{bmatrix} T \\ i_1 S \\ i_2 S \\ \vdots \\ i_{r-1} S \end{bmatrix}.
$$

There exists a unique $(c_1, \dots, c_r)$ satisfying above equation, as the matrix

$$
\begin{bmatrix} \tau & \xi_{20} & \xi_{30} & \cdots & \xi_{r0} \\ 0 & \sigma & \xi_{31} & \cdots & \xi_{r1} \\ 0 & 0 & \sigma & \cdots & \xi_{r2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma \end{bmatrix},
$$

having determinant $\tau\sigma^{r-1} > 0$, is invertible. This proves that the intersection between U and $\mathcal{P}^{i_1,\ldots,i_{r-1}}$ exists and is unique. □

Next, we show that each U_k must intersect at least $M^{r-2}+1$ hyper-balls in an optimal solution.

Proposition 12. *Let $\delta = \min_{i,j\in\{1,\ldots,\bar{N}\}} \frac{1}{2}\|\bar{x}_i - \bar{x}_j\|$ be the half of the minimum distance between two data points in the K-means instance. Suppose $M > 4\bar{N}^2d^2/\delta^2$, and M, S, T have sizes that is polynomial in N, K and D. If there exists U_k who intersect at most M^{r-2} hyper-balls in a solution $(\mathcal{C},\mathcal{U})$, then there is a polynomial time algorithm that finds a replacement of U_k, the subspace $U_k' \in \mathbb{R}^{D\times r}$, such that the KSS objective is strictly increased, where U_k' intersects all the hyper-balls.*

Proof. Recall that for each datum $\bar{x}_n$ in the K-means instance, we have constructed M^{r-1} data $X_n = \{x_n^{i_1,\ldots,i_{r-1}}\}$. Given the solution $\mathcal{U} = \{U_1,\ldots,U_K\}$ we are considering, we say a datum $x_n^{i_1,\ldots,i_{r-1}}$ is *covered* if there exists U_k such that the distance between $x_n^{i_1,\ldots,i_{r-1}}$ and U_k is less than δ: $\|x_n^{i_1,\ldots,i_{r-1}} - U_kU_k^\top x_n^{i_1,\ldots,i_{r-1}}\| < \delta$. As a result, if a datum is uncovered, it contributes at least δ^2 to the KSS objective.

Firstly, we show that there exists $n \in \{1,\ldots,\bar{N}\}$ such that X_n contains at least $\frac{\bar{N}-K}{\bar{N}}M^{r-1}$ uncovered data[1]. To see this, $\{X_n : n = 1,\ldots,\bar{N}\}$ form an equal-sized partition of all the $N = M^{r-1}\bar{N}$ data. By Proposition 9 and our definition of δ, each subspace that intersects at least $M^{r-2}+1$ balls can at most cover a single datum in each ball. Let K_1 be the number of subspaces that intersect at least $M^{r-2}+1$ balls, and let $K_2 = K - K_1$ be the number of subspaces that intersect at most M^{r-2} balls. The total number of covered data is at most

$$K_1M^{r-1}\cdot 1 + K_2M^{r-2}\cdot\bar{N} \le KM^{r-1}.$$

By the pigeonhole principle, there exists X_n that contains at most $\frac{KM^{r-1}}{\bar{N}}$ covered data, which implies our claim. Let X_{n^*} be such a partition.

Next, we show that the subspace that contains all the M^{r-1} data in X_{n^*}, which is

$$U_k' = \begin{bmatrix} \frac{\bar{x}_{n^*}}{\sqrt{\|\bar{x}_{n^*}\|^2+T^2}} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \frac{T}{\sqrt{\|\bar{x}_{n^*}\|^2+T^2}} & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix},$$

satisfies the requirement in the proposition (it is easy to see that U_k' is orthonormal and $U_k'(U_k')^\top x_{n^*}^{i_1,\ldots,i_{r-1}} = x_{n^*}^{i_1,\ldots,i_{r-1}}$). When replacing U_k by U_k' for certain U_k that intersects at

[1] It is reasonable to assume $\bar{N} > \bar{K} = K$ in the K-means instance, for otherwise the K-means instance is trivial: just let all the data be the centers.

most M^{r-2} balls, the loss in the objective function is at most $M^{r-2}\bar{N} \cdot 4d^2$ (even assuming U_k contains all the $M^{r-2}\bar{N}$ data in those M^{r-2} balls it intersects, these data can be assigned to U'_k with cost at most $(2d)^2$ as U'_k now intersects all the hyper-balls), and the increment in the objective function is at least $\frac{\bar{N}-K}{\bar{N}} M^{r-1} \cdot \delta^2 \geq \frac{1}{\bar{N}} M^{r-1}\delta^2$ (those $\frac{\bar{N}-K}{\bar{N}} M^{r-1}$ data not covered, each of which contributing at least δ^2 to the KSS objective, will have zero contribution if U'_k replaces U_k). By our assumption $M > 4\bar{N}^2 d^2/\delta^2$, the benefit of replacing U_k by U'_k is more than the loss.

Finally, to conclude the proof, it is obvious that finding such U'_k requires polynomial time. □

The proposition below is an extension of Lemma 6 to higher dimension, which says that the distance between $x \in \mathcal{S}^{i_1,\dots,i_{r-1}}$ and the subspace U is close to the distance between x and the intersection s of $\mathcal{S}^{i_1,\dots,i_{r-1}}$ and U. The former distance corresponds to the KSS objective, while the latter distance corresponds to the K-means objective if viewing all data in $\mathcal{S}^{i_1,\dots,i_{r-1}}$ as a K-means instance and s as a center.

Proposition 13. *Let $U \in \mathbb{R}^{D\times r}$ be a subspace that intersects at least $M^{r-2}+1$ hyper-balls. Fix an arbitrary hyperplane $\mathcal{P} := \mathcal{P}^{i_1,\dots,i_{r-1}}$, and let $s \in \mathbb{R}^D$ be the unique intersection between $\mathcal{P}$ and U (Corollary 11). For any $\zeta > 0$, there exists $\Pi > 0$ that depends only on ζ, r and d such that for any $x \in \mathcal{S}^{i_1,\dots,i_{r-1}}$, any $M \geq \Pi$, $S = M(r(2d+1)^3 + 2rMd^2)$, and $T = MS$, we have*

$$1 \leq \frac{\|x - s\|}{\|x - UU^\top x\|} \leq 1 + \zeta.$$

Proof. Proposition 10 shows that $U = [u_1 \quad \cdots \quad u_r]$, where $u_1, \dots, u_r$ are as defined in the statement of Proposition 10. The left part of the inequality is trivial, as the point in U that is closest to x is precisely x's projection on U, namely, $UU^\top x$. Thus, it remains to show the right part. By the definition of limit, this is equivalent as

$$\lim \frac{\|x - s\|}{\|x - UU^\top x\|} = 1 \qquad \text{or} \qquad \lim \|x - s\| = \lim \left\| x - UU^\top x \right\|,$$

where all the limits above, as well as all the limits in this proof, are taken over $M \to \infty$ while fixing $S = M(r(2d+1)^3 + 2rMd^2)$ and $T = MS$. It is important to notice that the limiting behavior should not depend on $\bar{D}$, as Π can only depend on ζ, r and d (it can depend on D, as $D = \bar{D} + r$ is dependent on r). We will make sure this is true, by ensuring our evaluation of the limit based solely on the upper bounds of those $\|\kappa_i\|$'s and $|\xi_{ij}|$'s given in Proposition 10. In particular, although the dimension of κ_i's depends on (in fact, is exactly) $\bar{D}$, but the bounds of their 2-norms, which is $\frac{rMd}{T}$ for κ_1 and $\frac{2d+1}{S}$ for remaining κ_i, do not depend on $\bar{D}$.

Since $|\|x - s\| - \|x - UU^\top x\|| \leq \|s - UU^\top x\|$, it suffices to show that $\lim \|s - UU^\top x\| = 0$. Let $B = [\kappa_1 \quad \cdots \quad \kappa_r] \in \mathbb{R}^{\bar{D}\times r}$, $\bar{x} \in \mathbb{R}^{\bar{D}}$ be the first $\bar{D}$ coordinates of

x, $\underline{x} = [T \quad i_1 S \quad \cdots \quad i_{r-1} S]$ be the last r coordinate of x, and

$$A = \begin{bmatrix} \tau & \xi_{20} & \xi_{30} & \cdots & \xi_{r0} \\ 0 & \sigma & \xi_{31} & \cdots & \xi_{r1} \\ 0 & 0 & \sigma & \cdots & \xi_{r2} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sigma \end{bmatrix},$$

so we have

$$U = \begin{bmatrix} B \\ A \end{bmatrix} \qquad \text{and} \qquad x = \begin{bmatrix} \bar{x} \\ \underline{x} \end{bmatrix}.$$

We express $UU^\top x$ and s in terms of $A, B, \bar{x}$ and $\underline{x}$. It is easy to compute $UU^\top x$:

$$UU^\top x = \begin{bmatrix} BB^\top & BA^\top \\ AB^\top & AA^\top \end{bmatrix} \begin{bmatrix} \bar{x} \\ \underline{x} \end{bmatrix} = \begin{bmatrix} BB^\top \bar{x} + BA^\top \underline{x} \\ AB^\top \bar{x} + AA^\top \underline{x} \end{bmatrix}.$$

For s, recall that $s = \sum_{j=1}^r c_j u_j$ where $c_1, \ldots, c_j$ satisfies

$$c_1 \begin{bmatrix} \tau \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} \xi_{20} \\ \sigma \\ 0 \\ \vdots \\ 0 \end{bmatrix} + c_3 \begin{bmatrix} \xi_{30} \\ \xi_{31} \\ \sigma \\ \vdots \\ 0 \end{bmatrix} + \cdots + c_r \begin{bmatrix} \xi_{r0} \\ \xi_{r1} \\ \xi_{r2} \\ \vdots \\ \sigma \end{bmatrix} = \begin{bmatrix} T \\ i_1 S \\ i_2 S \\ \vdots \\ i_{r-1} S \end{bmatrix},$$

which is

$$\begin{bmatrix} c_1 \\ \vdots \\ c_r \end{bmatrix} = A^{-1} \underline{x}.$$

Therefore, we have

$$s = U \begin{bmatrix} c_1 \\ \vdots \\ c_r \end{bmatrix} = \begin{bmatrix} B \\ A \end{bmatrix} A^{-1} \underline{x} = \begin{bmatrix} BA^{-1} \underline{x} \\ AA^{-1} \underline{x} \end{bmatrix}.$$

Putting together,

$$UU^\top x - s = \begin{bmatrix} BB^\top \bar{x} + BA^\top \underline{x} \\ AB^\top \bar{x} + AA^\top \underline{x} \end{bmatrix} - \begin{bmatrix} BA^{-1} \underline{x} \\ AA^{-1} \underline{x} \end{bmatrix} = UB^\top \bar{x} + U \left(A^\top - A^{-1} \right) \underline{x}.$$

To conclude the proposition, we will show

$$\lim \left\| UB^\top \bar{x} \right\| = 0 \qquad \text{and} \qquad \lim \left\| U \left(A^\top - A^{-1} \right) \underline{x} \right\| = 0.$$

It is easy to see the first limit by the Cauchy-Schwarz inequality:

$$\left\| UB^\top \bar{x} \right\| \leq \|U\|_F \|B^\top\|_F \|\bar{x}\|,$$

where $\|\cdot\|_F$ denotes the Frobenius norm. We have $\|U\|_F = \sqrt{r}$ (as the sum of the squares for each column of U is 1) and $\|\bar{x}\| \leq d$ (by our definition of d), which are both bounded. Moreover, by Proposition 10,

$$\lim \left\| B^\top \right\|_F^2 = \lim \left(\sum_{j=1}^{r} \|\kappa_j\|^2 \right) \leq \lim \left(\left(\frac{rMd}{T} \right)^2 + (r-1) \left(\frac{2d+1}{S} \right)^2 \right) = 0.$$

Therefore, we conclude the first limit.

It is a little bit more tricky to show the second limit, as $\|\underline{x}\|$ tends to infinity. By Cauchy-Schwarz inequality again, we have

$$\left\| U \left(A^\top - A^{-1} \right) \underline{x} \right\| \leq \|U\|_F \left\| \left(A^\top - A^{-1} \right) \underline{x} \right\|.$$

Since $\|U\|_F = \sqrt{r}$ is bounded, it remains to show that

$$\lim \left\| \left(A^\top - A^{-1} \right) \underline{x} \right\| = 0.$$

Let a_{ij} be the entry (i,j) of the matrix $A^\top - A^{-1}$. Noticing that $A^\top$ is lower-triangular and A^{-1} is upper-triangular, we have $a_{11} = \tau - \frac{1}{\tau}$, $a_{22} = \cdots = a_{rr} = \sigma - \frac{1}{\sigma}$, $a_{ij} = \xi_{i(j-1)}$ for all $i > j$, and a_{ij} is the entry (i,j) of A^{-1} for all $i < j$. We will show the limit by the following two steps.

1. We first show that $a_{i1} = o(\frac{1}{T})$ for all $i = 1, \ldots, r$, and $a_{ij} = o(\frac{1}{S})$ for all $i \neq j$ and $j \neq 1$. Since the first entry of $\underline{x}$ is T, and the remaining entries of $\underline{x}$ is $\Theta(S)$, noticing that r is a constant, this will imply

$$\lim \left\| \left(A^\top - A^{-1} \right) \underline{x} \right\|^2 = \lim \left((a_{11}T)^2 + \sum_{j=2}^{r} (a_{jj} i_{j-1} S)^2 \right).$$

2. In the second step, we show that the limit above is 0.

It is straightforward to show 2. Since Proposition 10 implies that $0 < 1 - \tau^2 < (\frac{rMd}{T})^2$ and $0 < 1 - \sigma^2 < (\frac{2d+1}{S})^2 + o(\frac{1}{S^2})$, we have

$$\lim |a_{11}T| = \lim \frac{(1-\tau^2)T}{\tau} \leq \frac{\lim \left(\frac{rMd}{T}\right)^2 T}{1} = r^2 d^2 \lim \frac{M^2}{T} = 0,$$

as $S = M(r(2d+1)^3 + 2rMd^2) > M^2 = \omega(M)$ and $T = MS = \omega(M^2)$. Similarly, for each $j = 2, \ldots, r$, we have

$$\lim |a_{jj} i_{j-1} S| = \lim \frac{(1-\sigma^2) i_{j-1} S}{\sigma} \leq \lim \left(\frac{2d+1}{S} \right)^2 i_{j-1} S = 0.$$

Putting together by noting that r is constant concludes 2.

To show 1, by noticing $S = \omega(M)$, Proposition 10 implies $a_{i1} = \xi_{i0} = \Theta(\frac{M}{ST}) = o(\frac{1}{T})$ and $a_{ij} = \xi_{i(j-1)} = \Theta(\frac{1}{S^2}) = o(\frac{1}{S})$ for all $i < j$. It remains to show that $a_{ij} = o(\frac{1}{S})$ for all $i > j$, which requires analysis on the upper-right part of the matrix A^{-1}.

Let A_d be the diagonal matrix whose diagonal entries are identical to A, and A_u be the strictly upper-triangular matrix whose upper-right part is identical to A, so that $A = A_d + A_u$. The calculation in [3] reveals that

$$A^{-1} = \left(\sum_{s=0}^{r} \left(-A_d^{-1} A_u \right)^s \right) A_d^{-1}.$$

Since $\tau^{-1} = \Theta(1)$ and $\sigma^{-1} = \Theta(1)$, the limit of A_d^{-1} is an identity matrix. Since the dimension of A is constant and the summation above also has constantly many terms, to analyze the asymptotic behavior of upper-right entries of A^{-1}, we can take $A^{-1} = \sum_{s=0}^{r} (-A_u)^s$. We know that each entry of A_u, which is certain ξ_{ij}, is $o(\frac{1}{S})$. Moreover, since the matrix has a constant dimension, it is easy to see that, if each entry in A_u^s is $o(\varsigma)$ for certain infinitesimal ς, then each entry in A_u^{s+1} is $o(\varsigma^2)$. As a result, we can conclude that each entry in the upper-right part of A^{-1} is $o(\frac{1}{S})$. Therefore, we conclude 2. $\square$

Finally, we are ready to prove Theorem 8. We show that, by choosing an arbitrary ζ with $0 < \zeta < \sqrt{1+\epsilon} - 1$ and letting $\varepsilon = \frac{1+\epsilon}{(1+\zeta)^2} - 1$, a $(1+\varepsilon)$-approximation polynomial time algorithm for the KSS problem implies a $(1+\epsilon)$-approximation polynomial time algorithm for the K-means problem.

Given a K-means instance, we construct the KSS instance based on our construction, with $M = \max\{4\bar{N}^2 d^2/\delta^2, \Pi\}$ where Π is given in Proposition 13, $S = M(r(2d+1)^3 + 2rMd^2)$, and $T = MS$. We first remark that the constructed KSS instance has a polynomial size. The reduction showing the APX-hardness of K-means in [1] satisfies $d = \delta = \sqrt{2}$.[2] Since $1/\zeta$ depends only on ϵ which is a constant, Π, depending only on $1/\zeta, r$ and d, is also a constant, so M is of polynomial size. Since r is a constant, S and T are of polynomial size as well. The total number of data, $N = M^{r-1}\bar{N}$, is also of polynomial size.

Suppose there is a $(1+\varepsilon)$-approximation polynomial algorithm for the KSS problem. We can assume without loss of generality that each U_k intersects at least $M^{r-2}+1$ hyperballs: if the algorithm output certain U_k fail to satisfy this, we can apply Proposition 12 to

[2]For a quick glance of the reduction in [1], the authors first show that the Vertex Cover problem on triangle-free graphs is APX-hard, then a datum $x_{ij} = e_i + e_j$ is constructed for each edge (i, j) with $1 \leq i, j \leq n$. Therefore, each data point only have two non-zero entries which equal to 1.

find a better replacement of each such U_k, which only takes extra polynomial time. By our construction, the K-means instance is duplicated to M^{r-1} copies such that each $\mathcal{S}^{i_1,\ldots,s_{r-1}}$ contains a copy, and the solution $\mathcal{U} = \{U_1, \ldots, U_K\}$ induces a K-means solution to each of these copies. In particular, for each $\mathcal{S}^{i_1,\ldots,i_{r-1}}$, each center s_k in the K-means problem is exactly the intersection of U_k and $\mathcal{P}^{i_1,\ldots,i_{r-1}}$ (Corollary 11 makes sure the intersection exists and is unique).

Given $\mathcal{U}$, let $\phi_{KSS}(\mathcal{U})$ be the KSS objective value for solution $(\mathcal{C},\mathcal{U})$, where $C_k \in \mathcal{C}$ consists of all data which are closest to U_k. Let $\phi_{KSS}^{i_1,\ldots,i_{r-1}}(\mathcal{U})$ be the contributions to the KSS objective value from all data in $\mathcal{S}^{i_1,\ldots,i_{r-1}}$, so that $\phi_{KSS}(\mathcal{U}) = \sum_{i_1,\ldots,i_{r-1}} \phi_{KSS}^{i_1,\ldots,i_{r-1}}(\mathcal{U})$. Let $\phi_{KM}^{i_1,\ldots,i_{r-1}}(\mathcal{U})$ be the K-means objective value for the K-means solution induced in the hyper-ball $\mathcal{S}^{i_1,\ldots,i_{r-1}}$. Let $\{s_1^*, \ldots, s_K^*\}$ (with $s_k^* \in \mathbb{R}^{\bar{D}}$) be an optimal solution to the K-means instance, and OPT_{KM} be the optimal objective value. Let $\mathcal{U}^* = \{U_1^*, \ldots, U_K^*\}$ where

$$U_k^* = \begin{bmatrix} \frac{s_k^*}{\sqrt{\|s_k^*\|^2+T^2}} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \frac{T}{\sqrt{\|s_k^*\|^2+T^2}} & 0 & 0 & \cdots & 0 \\ 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & 1 \end{bmatrix},$$

so $\mathcal{U}^*$ induces the same optimal solution in each of the M^{r-1} duplicated K-means instances.

By Proposition 13, we have

$$\phi_{KSS}^{i_1,\ldots,i_{r-1}}(\mathcal{U}^*) \le \phi_{KM}^{i_1,\ldots,i_{r-1}}(\mathcal{U}^*) \qquad \text{and} \qquad \phi_{KM}^{i_1,\ldots,i_{r-1}}(\mathcal{U}) \le (1+\zeta)^2 \phi_{KSS}^{i_1,\ldots,i_{r-1}}(\mathcal{U})$$

for each $i_1, \ldots, i_{r-1}$, and we also have

$$\phi_{KSS}(\mathcal{U}) \le (1+\varepsilon)\phi_{KSS}(\mathcal{U}^{OPT}) \le (1+\varepsilon)\phi_{KSS}(\mathcal{U}^*)$$

where $\mathcal{U}^{OPT}$ is an optimal solution to the constructed KSS instance. Putting together,

$$\begin{aligned} \sum_{i_1,\ldots,i_{r-1}} \phi_{KM}^{i_1,\ldots,i_{r-1}}(\mathcal{U}) &\le \sum_{i_1,\ldots,i_{r-1}} (1+\zeta)^2 \phi_{KSS}^{i_1,\ldots,i_{r-1}}(\mathcal{U}) \\ &= (1+\zeta)^2 \phi_{KSS}(\mathcal{U}) \\ &\le (1+\zeta)^2(1+\varepsilon)\phi_{KSS}(\mathcal{U}^*) \\ &= (1+\epsilon) \sum_{i_1,\ldots,i_{r-1}} \phi_{KSS}^{i_1,\ldots,i_{r-1}}(\mathcal{U}^*) \\ &\le (1+\epsilon) \sum_{i_1,\ldots,i_{r-1}} \phi_{KM}^{i_1,\ldots,i_{r-1}}(\mathcal{U}^*) \\ &= (1+\epsilon) M^{r-1} OPT_{KM}. \end{aligned}$$

This shows that, the *average* of the K-means objective values induced in all the duplicated instances is at most $(1+\epsilon)OPT_{KM}$. Therefore, we can exam the performances of the solutions induced in all those M^{r-1} identical K-means instance duplicates, and find the one with the best performance. This will gives a $(1+\epsilon)$-approximation to the K-means instance.

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