

# On Connections Between $k$ -Coloring and Euclidean $k$ -Means

Enver Aman

Rutgers University, Piscataway, NJ, USA

Karthik C. S.  

Rutgers University, Piscataway, NJ, USA

Sharath Punna

Rutgers University, Piscataway, NJ, USA

---

## Abstract

In the Euclidean  $k$ -means problems we are given as input a set of  $n$  points in  $\mathbb{R}^d$  and the goal is to find a set of  $k$  points  $C \subseteq \mathbb{R}^d$ , so as to minimize the sum of the squared Euclidean distances from each point in  $P$  to its closest center in  $C$ . In this paper, we formally explore connections between the  $k$ -coloring problem on graphs and the Euclidean  $k$ -means problem. Our results are as follows:

- For all  $k \geq 3$ , we provide a simple reduction from the  $k$ -coloring problem on regular graphs to the Euclidean  $k$ -means problem. Moreover, our technique extends to enable a reduction from a structured max-cut problem (which may be considered as a partial 2-coloring problem) to the Euclidean 2-means problem. Thus, we have a simple and alternate proof of the NP-hardness of Euclidean 2-means problem.
- In the other direction, we mimic the  $O(1.7297^n)$  time algorithm of Williams [TCS'05] for the max-cut of problem on  $n$  vertices to obtain an algorithm for the Euclidean 2-means problem with the same runtime, improving on the naive exhaustive search running in  $2^n \cdot \text{poly}(n, d)$  time.
- We prove similar results and connections as above for the Euclidean  $k$ -min-sum problem.

**2012 ACM Subject Classification** Theory of computation  $\rightarrow$  Problems, reductions and completeness; Theory of computation  $\rightarrow$  Complexity classes; Theory of computation  $\rightarrow$  Parameterized complexity and exact algorithms

**Keywords and phrases**  $k$ -means,  $k$ -minsum, Euclidean space, fine-grained complexity

**Digital Object Identifier** 10.4230/LIPIcs.ESA.2024.9

**Related Version** *Full Version:* <https://arxiv.org/abs/2405.13877>

**Funding** This work was supported by a grant from the Simons Foundation, Grant Number 825876, Awardee Thu D. Nguyen and by the National Science Foundation under Grant CCF-2313372.

**Acknowledgements** We would like to thank Pasin Manurangsi for pointing us to [6] and informing us that the fast max-sum convolution result of that paper can be used to obtain a  $2^n \cdot \text{poly}(n, d)$  runtime algorithm for the  $k$ -means problem. Also, we would like to thank Vincent Cohen-Addad for suggesting to us that the 2-min-sum problem might be more naturally connected to the Max-Cut problem. Finally, we would like to thank the anonymous reviewers for helping us improve the presentation of the paper.

## 1 Introduction

The  $k$ -means problem<sup>1</sup> is a classic objective for modelling clustering in a large variety of applications arising in data mining and machine learning. Given a set of  $n$  points  $P \subseteq \mathbb{R}^d$ , the goal is to find a set of  $k$  points  $C \subseteq \mathbb{R}^d$ , called *centers*, so as to minimize the sum of the

---

<sup>1</sup> Throughout this paper, we consider the  $k$ -means problem only in the Euclidean space.



squared distances from each point in  $P$  to its closest center in  $C$ . The algorithmic study of the  $k$ -means problem arguably started with the seminal work of Lloyd [29]. Since then, the problem has received a tremendous amount of attention [4, 40].

The  $k$ -means problem is known to be NP-Hard, even when the points lie in the Euclidean plane (and  $k$  is large) [30], or even when  $k = 2$  (and the dimension is large) [15]. On the positive side, a near linear time approximation scheme exists when the dimension is fixed (and the number of clusters  $k$  is arbitrary) [8], or when the number of clusters is constant (and the dimension  $d$  is arbitrary) [26, 5]. When both  $k$  and  $d$  are arbitrary, several groups of researchers have shown hardness of approximation results [2, 28, 9, 11].

### Fine-Grained Complexity

One of the main research directions in Fine-Grained Complexity is to identify the exact complexity of important hard problems, distinguishing, say, between NP-complete problems where exhaustive search is essentially the best possible algorithm, and those that have improved exponential time algorithms [36, 37, 38]. The importance of high-dimensional Euclidean inputs in statistics and machine learning applications has led researchers to study the parameterized and fine-grained complexity of the problem. Both the dimensionality of the input,  $d$ , and the target number of clusters,  $k$ , have been studied as parameters, in as early as the mid 90s.

The  $k$ -means problems can be solved in time  $O(k^n \cdot \text{poly}(n, d))$  by simply performing an exhaustive search over the solution space. This can be improved to  $4^n \cdot \text{poly}(n, d)$  runtime using dynamic programming [24], which itself can be further improved to  $2^n \cdot \text{poly}(n, d)$  runtime using fast max-sum convolution [6]. The seminal work of Inaba, Katoh, and Imai [23] has shown that one can compute an exact solution to the  $k$ -means problems in time  $n^{kd+1}$ . However, this algorithm clearly suffers from the so-called “curse of dimensionality”, the higher the dimension, the higher the running time. Thus, for high dimensions, say when  $d = n$ , the algorithm in [23] is slower than even the exhaustive search over the solution space. Therefore, we ask:

*Can we beat  $2^n$  runtime for  $k$ -means problem in high dimensions?<sup>2</sup>*

The complexity of  $k$ -means problem increases as the number of cluster  $k$  increases. Therefore, if the answer to the above question is in the affirmative, then a natural first step would be to try to beat the exhaustive search algorithm for 2-means problem.

*Is there an algorithm for 2-means problem running in time  $2^{(1-\varepsilon)n}$ , for some  $\varepsilon > 0$ ?*

Additionally, the case of  $k = 2$  for the  $k$ -means problem is of practical interest, for example, in medical testing to determine if a patient has certain disease or not, and industrial quality control to decide whether a specification has been met, and also in information retrieval to decide whether a page should be in the result set of a search or not.

Apriori, there is no reason to suspect that an improvement over exhaustive search is even possible, and one might instead be able to prove conditional lower bounds assuming one of the popular fine-grained complexity theoretic hypothesis such as the *Strong Exponential Time*

---

<sup>2</sup> In [20], the authors provide a better than  $2^n$  runtime algorithm (to be precise an  $1.89^n \text{poly}(n, d)$  runtime algorithm) for a *discrete* variant of the  $k$ -means problem, where the centers need to be picked from the input point-set. Their result extends to the discrete variant of the  $k$ -median and  $k$ -center problems as well. However, the discrete variant is not as natural as the continuous variant in geometric spaces.

*Hypothesis* [21, 22] or the *Set Cover Conjecture* [12]. In fact, over the last decade, there have been a large number of conditional lower bounds proven under these two assumptions ruling out algorithms which are faster than exhaustive search (for example, see [12, 32, 25, 1, 27]). Thus, it comes as a pleasant surprise that our main result is an affirmative answer to the above question on the 2-means problem.

► **Theorem 1.** *There is an exact algorithm for the 2-means problem running in time  $1.7297^n \cdot \text{poly}(n, d)$ , where  $n$  is the number of input points<sup>3</sup>.*

We remark that, under the hypothesis that the matrix multiplication constant  $\omega = 2$ , our runtime can be improved to  $1.59^n \cdot \text{poly}(n, d)$ .

From a technical point-of-view, the ideas and intuition behind our algorithm provide a lot of conceptual clarifications and insights, and we elaborate more on that below.

### Connection to Max-Cut Problem

There are a lot of connections between clustering problems and graph cut problems (for example, spectral clustering [33] or metric Max-Cut [16]). The popular graph cut problems that are motivated by geometric clustering tasks are (variants of) the min-cut problem and sparsest cut problem. Intuitively, in these two cut problems, a node corresponds to a point of a clustering problem, and an edge corresponds to similarity (i.e., proximity in the distance measure) between the corresponding points. Such a connection is presented in [17] to prove the NP-hardness of 2-median in  $\ell_1$ -metric.

One of the key insights, inspired by the embedding in [10, 18], is a connection between the Max-Cut problem and the (Euclidean) 2-means problem! In the Max-Cut problem, we are given as input a graph and the goal is to partition the vertex set into two parts such that the number of edges across the parts is maximized. We provide an intimate connection between Max-Cut (with some special guarantees) and 2-means by showing the following:

- In Section 3, we present a simple embedding of the vertices of a Max-Cut instance (with additional guarantees) into Euclidean space such that any clustering of the resulting pointset into two clusters minimizing the 2-means objective yields a partition of the vertices of the Max-Cut instance maximizing the number of edges across the parts. This gives an alternate view to [15] on the hardness of 2-means (see Remark 5 to know more about the technical differences).
- In [35], Williams designed an algorithm to solve Max-Cut in better than exhaustive search time. This algorithmic technique can be adopted for the 2-means problem to give us<sup>4</sup> Theorem 1. However, we have to take some additional care due to the geometric nature of the problem.

In fact, the structured Max-Cut instances that we identify are quite powerful – in Section 6, we show that the structured Max-Cut problem is computationally equivalent to 2-min-sum<sup>5</sup> problem under polynomial time reductions. This yields both hardness of 2-min-sum and also an  $1.7297^n \cdot \text{poly}(n, d)$  time algorithm for 2-min-sum (much like Theorem 1).

<sup>3</sup> In this theorem, we assume that the coordinate entries of all points in the input are integral and that the absolute value of any coordinate is bounded by  $2^{O(n)}$ .

<sup>4</sup> For the sake of ease of presentation, we use the more generalized algorithm of Williams for Weighted 2-CSPs given in [34].

<sup>5</sup>  $k$ -min-sum is another classic clustering objective and is defined in Section 2.

### Connection to $k$ -Coloring Problem

Moreover, in Section 4 we present a general and yet *simple* connection between  $k$ -coloring and  $k$ -means clustering for<sup>6</sup>  $k > 2$ . This yields an even simpler proof of NP-hardness of 3-means problems. Additionally, it opens up the below new research direction for future exploration:

There is an inclusion-exclusion based algorithm that runs in  $2^n \cdot \text{poly}(n, d)$  time for the  $k$ -coloring problem on  $n$  vertex graphs [7]. On the other hand, for fixed  $k$ , there are techniques different from William's technique [35] to beat the  $2^n \cdot \text{poly}(n)$  time algorithm for  $k$ -coloring problem [3, 19, 41].

*Can we use the algorithmic techniques developed for  $k$ -coloring to obtain similar runtimes for  $k$ -means (for small values of  $k$ )?*

Another important fine-grained complexity question is about beating exhaustive search for other popular clustering objectives.

*Is there an algorithm for Euclidean 2-center or 2-median problem running in time  $2^{(1-\varepsilon)n}$ , for some constant  $\varepsilon > 0$ ?*

## 1.1 Organization of the Paper

In Section 2, we formally introduce the problems of interest to this paper and also prove/recall some basic NP-hardness results. In Section 3, we provide a linear size blow up reduction from (a specially structured) Max-cut instance to the 2-means problem. In Section 4, we provide a linear time reduction from  $k$ -coloring problem to the  $k$ -means problem. In Section 5, we provide an algorithm for 2-means problem that beats exhaustive search. Finally, in Section 6, we prove the computational equivalence of 2-min-sum and (structured) Max-Cut problems.

## 2 Preliminaries

In this section, we define the clustering problems studied in this paper. We also define the graph problems and prove/recall their (known) hardness results for the sake of completeness.

### 2.1 Problem Definitions

#### $k$ -means clustering problem

The input is a set of  $n$  points  $P \subset \mathbb{R}^d$  and the output is a partition of points into clusters  $C_1, \dots, C_k$ , along with their centers  $\mu_1, \dots, \mu_k \in \mathbb{R}^d$  such that the following objective, the  $k$ -means cost, is minimized:

$$\sum_{j=1}^k \sum_{x \in C_j} \|x - \mu_j\|^2.$$

Here,  $\|\cdot\|$  is the Euclidean distance. In the decision version of the problem, a rational  $R$  will be given as part of the input, and the output is *YES* if there exists a partition such that its  $k$ -means cost is less than or equal to  $R$ , and *NO* otherwise. Moreover in the above

---

<sup>6</sup> It is appropriate to view Max-Cut as almost 2-coloring.

formulation of the objective, it can be shown that the *center*  $\mu_j$  of a cluster  $C_j$  is the centroid of the points in that cluster. Using this result,  $\mu_j$  can be removed from the above objective function and it simplifies to minimizing:

$$\sum_{j=1}^k \left( \frac{1}{2|C_j|} \cdot \sum_{x,y \in C_j} \|x - y\|^2 \right).$$

### ***k*-min-sum clustering problem**

Let  $(M, d)$  be a metric space. The input is a set of  $n$  points  $X \subseteq (M, d)$  and the output is a partition of points into clusters  $C_1, \dots, C_k$  such that the following objective, the *k-min-sum cost*, is minimized:

$$\sum_{j=1}^k \sum_{x,y \in C_j} d(x, y),$$

where  $d(\cdot, \cdot)$  is the metric distance measure. In the decision version, an integer  $Z$  will be given as the part of the input, and the output is *YES* if there exists a partition such that its *k-min-sum cost* is less than or equal to  $Z$ , and *NO* otherwise.

In this paper, we study the *k-means* problem in Euclidean space, but we study the *k-min-sum* problem in general metric.

### **Balanced Max-Cut problem**

The input is a  $d$ -regular graph  $G = (V, E)$  and an integer  $t$ . For any partition of  $V$  into two parts, an edge is called a *bad edge* if both of its vertices are in the same part and is a *good edge* otherwise. The problem is to distinguish between the following two cases:

- *YES instance*: There exists a balanced cut of  $V$  into  $V_0 \dot{\cup} V_1$ , such that  $|V_0| = |V_1|$  and the total number of bad edges is equal to  $t$ .
- *NO instance*: For every 2-partition of  $V$  into  $V_0 \dot{\cup} V_1$ , the total number of bad edges is strictly greater than  $t + \frac{t}{|V|} \cdot \left| |V_0| - |V_1| \right|$ .

Note that this problem is slightly different from the conventional way of defining the *Max-Cut* problem in two ways. The partition sets  $V_0$  and  $V_1$  need to be of same size in the *YES* case, and we focus on the bad edges instead of the edges cut (although it is still a *Max-Cut* problem due to the regularity of the input graph).

### ***k*-coloring problem (on regular graphs)**

The input is a  $d$ -regular graph  $G = (V, E)$  and an integer  $k$  and the output is *YES*, if there exists a  $k$ -coloring of the vertices of the graph such that no two adjacent vertices are of the same color; else, the output is *NO*.

### **NAE-3-SAT problem**

The input is a collection of  $m$  clauses on  $n$  variables. Each clause contains three variables or negation of variables. The output is *YES* if and only if there exists an assignment of the variables such that all three values in every clause are not equal to each other. In other words, every clause has at least one true value and at least one is false.

### Weighted 2-CSP

The input are integers  $K_v, K_e \in [N^\ell]^+$  for a fixed integer  $\ell > 0$  independent of the input, a finite domain  $D$ , and functions:

$$w_i : D \rightarrow [N^\ell]^+, \forall i = 1, \dots, N, \quad w_{(i,j)} : D \times D \rightarrow [N^\ell]^+, \forall i, j = 1, \dots, N, \text{ such that } i < j,$$

where  $[N^\ell]^+ := \{0, 1, \dots, N^\ell\}$ . The output to the Weighted 2-CSP problem is *YES* if and only if there is a variable assignment  $a = (a_1, \dots, a_N) \in D^N$  such that,

$$\sum_{i \in [N]} w_i(a_i) = K_v, \quad \sum_{\substack{i, j \in [N] \\ i < j}} w_{(i,j)}(a_i, a_j) = K_e.$$

## 2.2 Computational Hardness of Graph Problems

In this subsection, we state the NP-hardness of *Balanced Max-Cut* and *k-coloring*.

► **Theorem 2** ([13]). *k-coloring is NP-Hard for all  $k > 2$ .*

► **Theorem 3.** *Balanced Max-Cut is NP-Hard.*

The proof of the above theorem is a reduction from an NP-hard structured variant of NAE-3-SAT problem and is deferred to Appendix A.

### 3 Reduction from Balanced Max-Cut to 2-means

In this section, we give a (linear size blow up) reduction from *Balanced Max-Cut* to *2-means* problem.

#### Construction

Let  $(G = (V, E), t)$  be the input to an instance of the Balanced Max-Cut problem where  $G$  is a  $d$ -regular graph. Let  $n := |V|$  and  $m := |E|$ . We build  $n$  points in  $\mathbb{R}^m$  and set the task of checking if the 2-means cost is equal to  $nd - 2d + 4t/n$ . Arbitrarily orient the edges of the graph  $G$ . For every  $v \in V$ , we have a point  $p_v \in \mathbb{R}^m$  in the point-set where  $\forall e \in [m]$ ,

$$p_v(e) = \begin{cases} +1 & \text{if } e \text{ is outgoing from } v, \\ -1 & \text{if } e \text{ is incoming to } v, \\ 0 & \text{otherwise.} \end{cases}$$

▷ **Claim 4.** For any two-partition of  $V := V_1 \dot{\cup} V_2$ , let the number of bad edges in each part be  $r_1, r_2$  respectively. Then, the 2-means cost of the corresponding 2-clustering  $C_1, C_2$  is given by  $nd - 2d + 2 \sum_{j=1}^2 \frac{r_j}{|V_j|}$ .

*Proof.* Fix  $j \in \{1, 2\}$ . Let us begin by computing the center of a cluster  $C_j$ . Observe that a good edge  $e$  contributes a  $\pm \frac{1}{|C_j|}$  additive factor to the center on the  $e^{th}$  coordinate, whereas a bad edge contributes nothing. So, the center of a cluster  $C_j$  is given by the following expression:

$$c_j(e) = \frac{1}{|C_j|} \cdot \sum_{p_v \in C_j} p_v(e) = \begin{cases} \frac{1}{|C_j|} & \text{if } e \text{ is good edge and } \exists p_v \in C_j \text{ s.t. } p_v(e) = 1, \\ -\frac{1}{|C_j|} & \text{if } e \text{ is good edge and } \exists p_v \in C_j \text{ s.t. } p_v(e) = -1, \\ 0 & \text{otherwise.} \end{cases}$$

For any  $v \in V_j$ , the cost contributed by a good edge  $e$  is given by:

$$|p_v(e) - c_j(e)| = \begin{cases} 1 - \frac{1}{|C_j|} & \text{when } v \in e \text{ and } c_j(e) \neq 0, \\ \frac{1}{|C_j|} & \text{when } v \notin e \text{ and } c_j(e) \neq 0, \\ 0 & \text{otherwise.} \end{cases}$$

The cost contributed by a bad edge  $e$  is given by

$$|p_v(e) - c_j(e)| = \begin{cases} 1 & \text{when } |p_v(e)| = 1, \\ 0 & \text{otherwise.} \end{cases}$$

We rewrite the  $\mathcal{L}$ -means cost in terms of cost contributed by good and bad edges as follows:

$$\begin{aligned} \sum_{j=1}^2 \sum_{p_v \in C_j} \|p_v - c_j\|^2 &= \sum_{j=1}^2 \sum_{p_v \in C_j} \sum_{e \in E} |p_v(e) - c_j(e)|^2 = \sum_{j=1}^2 \sum_{e \in E} \sum_{p_v \in C_j} |p_v(e) - c_j(e)|^2 \\ &= \sum_{j=1}^2 \left[ \sum_{e \text{ is good}} \sum_{p_v \in C_j} |p_v(e) - c_j(e)|^2 + \sum_{e \text{ is bad}} \sum_{p_v \in C_j} |p_v(e) - c_j(e)|^2 \right] \end{aligned}$$

The cost contributed by a bad edge in a cluster  $C_j$  is given by:  $\sum_{p_v \in C_j} |p_v(e) - c_j(e)|^2 = 1 \cdot 2 + (|C_j| - 2) \cdot 0 = 2$ , and there are  $r_j$  many such bad edges. On the other hand, the cost contributed by a good edge on all vertices in the cluster  $C_j$  is  $\sum_{p_v \in C_j} |p_v(e) - c_j(e)|^2 = (1 - \frac{1}{|C_j|})^2 + (\frac{1}{|C_j|})^2 \cdot (|C_j| - 1) = (1 - \frac{1}{|C_j|})$ , and there are  $|C_j|d - 2r_j$  many good edges in each part. Putting it together, the total  $\mathcal{L}$ -means cost:

$$\sum_{j=1}^2 \left[ 2r_j + (|C_j|d - 2r_j) \cdot \left(1 - \frac{1}{|C_j|}\right) \right] = nd - 2d + 2 \sum_{j=1}^2 \frac{r_j}{|C_j|}. \quad \triangleleft$$

### Completeness

In an *YES* instance,  $|C_1| = |C_2| = \frac{n}{2}$  and  $r_1 + r_2 = t$ . So, from Claim 4, the  $\mathcal{L}$ -means cost is:

$$nd - 2d + 2 \frac{r_1 + r_2}{n/2} = nd - 2d + 4t/n.$$

### Soundness

In a *NO* instance,  $|C_1| + |C_2| = n$  and  $r_1 + r_2 > t + \frac{t}{n} \cdot (|C_1| - |C_2|)$ .

Assume, for the sake of contradiction, there exists a clustering  $C_1, C_2$  such that its  $\mathcal{L}$ -means cost is  $\leq nd - 2d + 4t/n$ . From Claim 4, this implies:

$$\frac{r_1}{|C_1|} + \frac{r_2}{|C_2|} \leq \frac{2t}{n}. \quad (1)$$

Without loss of generality let us suppose that  $|C_1| \geq |C_2|$ , and thus let  $c := |C_1|$  and  $\delta := |C_1| - |C_2| \geq 0$ . We may assume that  $\delta > 0$ , because otherwise, we immediately arrive at a contradiction as the soundness assumption tells us that  $r_1 + r_2 > t$  and (1) implies that  $r_1 + r_2 \leq t$ .

We can now rewrite (1) as follows:

$$n \cdot (c - \delta) \cdot (r_1 + r_2) + \delta nr_2 \leq c \cdot (c - \delta) \cdot 2t.$$

## 9:8 On Connections Between $k$ -Coloring and Euclidean $k$ -Means

Combining the above with the soundness assumption that  $r_1 + r_2 > t(1 + \delta/n)$  and that  $n = 2c - \delta$ , we obtain:

$$\delta nr_2 < (c - \delta) \cdot t \cdot (2c - n - \delta) = 0.$$

Since both  $\delta$  and  $n$  are positive, this implies  $r_2 < 0$ , which is a contradiction. This completes the soundness analysis of the reduction.

► **Remark 5.** The starting point of the proof of NP-hardness of 2-means given in [15] is also NAE-3-SAT (much like the starting point of the NP-hardness proof idea of Balanced Max-Cut). However, in [15], the authors directly construct the distance matrix of the input points from the NAE-3-SAT instance and then argue that the distance matrix can indeed be realized in  $\ell_2^2$ . On the other hand, our proof sheds new light by identifying a clean graph theoretic intermediate problem, namely the Balanced Max-Cut problem, which then admits a very simple embedding to the Euclidean space.

### 4 Reduction from $k$ -Coloring to $k$ -means

In this section, we sketch a (linear size blow up) reduction from  $k$ -coloring to  $k$ -means problem. Invoking Theorem 2 then gives an alternate proof of NP-hardness for the  $k$ -means problem when  $k \geq 3$ .

#### Construction

Let  $(G = (V, E), k)$  be the input to an instance of the  $k$ -coloring problem where  $G$  is a  $d$ -regular graph. Let  $n := |V|$  and  $m := |E|$ . We build the point set  $P$  of  $n$  points in  $\mathbb{R}^m$  and set the  $k$ -means cost equal to  $nd - kd$ . Arbitrarily orient the edges of the graph  $G$ . For every  $v \in V$ , we have a point  $p_v \in \mathbb{R}^m$  where  $\forall e \in [m]$ ,

$$p_v(e) = \begin{cases} +1 & \text{if } e \text{ is outgoing from } v, \\ -1 & \text{if } e \text{ is incoming to } v, \\ 0 & \text{otherwise.} \end{cases}$$

The proof of the completeness and soundness follows in a similar (actually much simpler) way to that of Section 3.

### 5 An $1.7297^n \cdot \text{poly}(n, d)$ runtime Algorithm for 2-means

In this section, we discuss the algorithm that beats exhaustive search for the 2-means problem. The key idea of the algorithm is to reduce the given 2-means instance to a *Weighted 2-CSP* instance (see Section 2 for its definition). Then we use the matrix multiplication based fast algorithm for the Weighted 2-CSP problem<sup>7</sup> to beat the  $2^n$  time bound for 2-means problem. Formally, we prove the following theorem.

► **Theorem 6.** *There is an exact algorithm for the 2-means problem running in time  $2^{\omega n/3} \cdot \text{poly}(n, d)$ , where  $n$  is the number of input points,  $d$  is the dimensionality of the Euclidean space, and  $\omega$  is the matrix multiplication constant.*

---

<sup>7</sup> This is a generalization of the max-cut problem [34].



► **Corollary 7.** *There is an exact algorithm for the 2-means problem running in time  $O(1.7297^n)$ .*

**Proof.** By using the best known value of matrix multiplication constant,  $\omega = 2.371552$  [39], we upper bound the time complexity in Theorem 6 by  $1.7297^n \cdot \text{poly}(n, d)$ . ◀

To prove Theorem 6, we need the well-known algorithm of Williams [34] which in turns relies on the algorithm of Nešetřil and Poljak, [31] to quickly detect a  $k$ -clique in a graph via Matrix Multiplication.

► **Theorem 8** (Theorem 6.4.1 in [34]<sup>8</sup>). *Weighted 2-CSP instances with weights in  $[N^\ell]^+$  are solvable in*

$$N^{O(\ell)} + 27 \cdot |D|^{\omega N/3} \text{ time,}$$

where  $N$  is the number of variables,  $D$  is the domain, and  $\omega$  is the matrix multiplication constant.

We are now ready to prove Theorem 6. For the sake of presentation, we will assume that the coordinate entries of all points in the input are integral and that the absolute value of any coordinate is bounded by  $\text{poly}(n, d)$  (although our claims would go through even if the absolute value of any coordinate is bounded above by  $2^{o(n)}$ ). Moreover, we will assume that  $d = n^{O(1)}$ .

**Proof of Theorem 6.** For the ease of presentation, assume  $n$  is divisible by 3. Let  $P$  be the set of given input points to the 2-means instance (where  $|P| = n$ ). Under the assumption that the input is integral, let the largest absolute value of any coordinate appearing in  $P$  be  $M$ . Then, the squared Euclidean distance between any two points  $x, y \in P$  is bounded by

$$\|x - y\|^2 = \sum_{i=1}^d |x_i - y_i|^2 \leq \sum_{i=1}^d (2M)^2 = 4M^2d.$$

Consequently, we obtain that, for any partition of  $P$  to  $A$  and  $B$ , we have:

$$\begin{aligned} \left( |B| \cdot \sum_{x, y \in A} \|x - y\|^2 \right) + \left( |A| \cdot \sum_{x, y \in B} \|x - y\|^2 \right) &\leq (|A| \cdot |B|^2 + |B| \cdot |A|^2) \cdot 4M^2d \\ &\leq 8M^2n^3d < n^\ell, \end{aligned}$$

for some fixed constant  $\ell$  (for large enough  $n$ ).

Arbitrarily partition  $P$  into 3 sets  $P_1, P_2$ , and  $P_3$  with  $n/3$  points in each set. For every  $\mathbf{K} := (K_v, K_e) \in \mathbb{Z}_{\geq 0}^2$  such that  $K_v + K_e \leq n^\ell$ , and  $\mathbf{ab} := (a_1, a_2, a_3, b_1, b_2, b_3) \in \mathbb{Z}_{\geq 0}^6$ , such that  $a_1 + a_2 + a_3 + b_1 + b_2 + b_3 = n$ , we construct an instance  $\Phi_{\mathbf{ab}, \mathbf{K}}$  of Weighted 2-CSP on 3 variables  $v_1, v_2$ , and  $v_3$  as follows.

For every  $i \in [3]$ , let  $D_i := \{(P_i^A, P_i^B) : P_i^A \cup P_i^B = P_i, P_i^A \cap P_i^B = \emptyset, |P_i^A| = a_i, |P_i^B| = b_i\}$ . Let  $D := D_1 \cup D_2 \cup D_3$  be the domain of  $\Phi_{\mathbf{ab}, \mathbf{K}}$ . Note that  $|D| \leq 3 \cdot 2^{n/3}$ . It remains to define the weight functions  $w_1, w_2, w_3, w_{(1,2)}, w_{(2,3)}, w_{(1,3)}$  to complete the construction of  $\Phi_{\mathbf{ab}, \mathbf{K}}$ .

<sup>8</sup> We set  $k(n)$  to be the constant function always equal to 3 in Theorem 6.4.1 of [34]. Additionally, the definition of weighted 2-CSP in [34] distinguishes the constraint  $(i, j)$  from the constraint  $(j, i)$ , for all  $i, j \in [N]$ ,  $i \neq j$ . In this paper, we work with the simpler  $\{i, j\}$  instead.

**9:10 On Connections Between  $k$ -Coloring and Euclidean  $k$ -Means**

For every  $i \in [3]$  and every  $(P_i^A, P_i^B) \in D_i$ , we define:

$$w_i((P_i^A, P_i^B)) := (b_1 + b_2 + b_3) \cdot \left( \sum_{x, y \in P_i^A} \|x - y\|^2 \right) + (a_1 + a_2 + a_3) \cdot \left( \sum_{x, y \in P_i^B} \|x - y\|^2 \right).$$

For every  $a \in D \setminus D_i$ , we define  $w_i(a) := K_v + 1$ .

Next, for every  $i, j \in [3]$  such that  $i < j$ , and every  $(P_i^A, P_i^B) \in D_i$  and  $(P_j^A, P_j^B) \in D_j$ , we define:

$$w_{(i,j)}((P_i^A, P_i^B), (P_j^A, P_j^B)) := (b_1 + b_2 + b_3) \cdot \left( \sum_{\substack{x \in P_i^A \\ y \in P_j^A}} \|x - y\|^2 \right) + (a_1 + a_2 + a_3) \cdot \left( \sum_{\substack{x \in P_i^B \\ y \in P_j^B}} \|x - y\|^2 \right).$$

For every  $(a, a') \in D \times D \setminus D_i \times D_j$ , we define  $w_{(i,j)}(a, a') := K_e + 1$ .

Recall, that the output to  $\Phi_{\mathbf{ab}, \mathbf{K}}$  must be *YES* if and only if

$$\sum_{i \in [3]} w_i(a_i) = K_v, \quad \sum_{\substack{i, j \in [3] \\ i < j}} w_{(i,j)}(a_i, a_j) = K_e.$$

Also note that the number of weighted 2-CSP instances we constructed is  $\text{poly}(n)$ , and the construction time of each instance is at most  $\tilde{O}(D^2) = 2^{2n/3} \cdot \text{poly}(n, d)$ .

We run the algorithm in Theorem 8 on all the above constructed Weighted 2-CSP instances, and let  $\Phi_{\mathbf{ab}, \mathbf{K}}^*$  be an instance whose output is *YES*, and for which  $\frac{K_e + K_v}{(a_1 + a_2 + a_3) \cdot (b_1 + b_2 + b_3)}$  is minimized (amongst all instances for which the algorithm outputted *YES*; it is easy to observe that there is at least one instance whose output by the algorithm is *YES*).

Let  $((P_1^A, P_1^B), (P_2^A, P_2^B), (P_3^A, P_3^B))$  be the variable assignment to  $\Phi_{\mathbf{ab}, \mathbf{K}}^*$  which satisfies all the constraints. Then we claim that the two clusters  $P^A := P_1^A \cup P_2^A \cup P_3^A$  and  $P^B := P_1^B \cup P_2^B \cup P_3^B$  minimizes the 2-means objective for  $P$ . We prove this by contradiction as follows.

Suppose (one of) the minimizers of the 2-means objective for  $P$  is given by the clustering  $Q^A \dot{\cup} Q^B = P$ . For the sake of contradiction, we assume that the 2-means cost of  $Q^A \dot{\cup} Q^B$  is strictly less than the 2-means cost of  $P^A \dot{\cup} P^B$ , i.e.,

$$\begin{aligned} & \left( \frac{1}{|Q^A|} \cdot \sum_{x, y \in Q^A} \|x - y\|^2 \right) + \left( \frac{1}{|Q^B|} \cdot \sum_{x, y \in Q^B} \|x - y\|^2 \right) \\ & < \left( \frac{1}{|P^A|} \cdot \sum_{x, y \in P^A} \|x - y\|^2 \right) + \left( \frac{1}{|P^B|} \cdot \sum_{x, y \in P^B} \|x - y\|^2 \right) \end{aligned} \quad (2)$$

For every  $i \in [3]$ , let  $Q_i^A := P_i \cap Q^A$  and  $Q_i^B := P_i \cap Q^B$ . Let  $\tilde{\mathbf{ab}} := (|Q_1^A|, |Q_2^A|, |Q_3^A|, |Q_1^B|, |Q_2^B|, |Q_3^B|)$  and let  $\tilde{\mathbf{K}} := (\tilde{K}_v, \tilde{K}_e)$  where  $\tilde{K}_v$  and  $\tilde{K}_e$  are defined as follows:

$$\begin{aligned} \tilde{K}_v &:= \sum_{i \in [3]} \left( |Q^B| \cdot \left( \sum_{x, y \in Q_i^A} \|x - y\|^2 \right) + |Q^A| \cdot \left( \sum_{x, y \in Q_i^B} \|x - y\|^2 \right) \right), \\ \tilde{K}_e &:= \sum_{\substack{i, j \in [3] \\ i < j}} \left( |Q^B| \cdot \left( \sum_{\substack{x \in Q_i^A \\ y \in Q_j^A}} \|x - y\|^2 \right) + |Q^A| \cdot \left( \sum_{\substack{x \in Q_i^B \\ y \in Q_j^B}} \|x - y\|^2 \right) \right). \end{aligned}$$

By construction, we have that  $((Q_1^A, Q_1^B), (Q_2^A, Q_2^B), (Q_3^A, Q_3^B))$  is an assignment to  $\Phi_{\mathbf{a}\bar{\mathbf{b}}, \tilde{\mathbf{K}}}$  that satisfies all the constraints.

However from (2), note that:

$$\frac{K_e + K_v}{|P^A| \cdot |P^B|} > \frac{\tilde{K}_e + \tilde{K}_v}{|Q^A| \cdot |Q^B|},$$

leading to a contradiction. ◀

## 6 Fine-Grained Complexity of 2-min-sum

In this section, we study the fine-complexity of the *2-min-sum* problem in general  $\ell_p$ -metric spaces.

► **Theorem 9.** *The 2-min-sum and Balanced Max-Cut problems are computationally equivalent in  $\ell_p$ -metrics:*

- Given a 2-min-sum instance, there is a polytime algorithm to reduce it to a weighted Max-Cut instance.
- Given a Balanced Max-Cut instance, there is a polytime algorithm to reduce it to a 2-min-sum instance.

### 6.1 Reduction from Balanced Max-Cut to 2-min-sum

In this subsection, we give a reduction from *Balanced Max-Cut* as defined in Section 2 (and thus the NP-hardness in Theorem 3 applies to 2-min-sum as well).

#### Reduction to 2-min-sum in $\ell_p$ -metric

Let  $G = (V, E)$  and  $t > 0$  be an instance to the *Balanced Max-Cut* problem. Let  $n = |V|$  and  $m = |E|$ . We build  $n$  points in  $\mathbb{R}^m$  and set the *2-min-sum* cost equal to

$$\alpha_{n,p,d,t} := (2d)^{1/p} \left( \frac{n^2 - 2n}{4} \right) + t[(2d + 2^p - 2)^{1/p} - (2d)^{1/p}].$$

Arbitrarily orient the edges of the graph  $G$ . For every  $v \in V$ , we define a point  $p_v \in \mathbb{R}^m$  in the point-set where  $\forall e \in [m]$ ,

$$p_v(e) = \begin{cases} +1 & \text{if } e \text{ is outgoing from } v, \\ -1 & \text{if } e \text{ is incoming to } v, \\ 0 & \text{otherwise.} \end{cases}$$

▷ **Claim 10.** For any two-partition of  $V = V_1 \dot{\cup} V_2$ , let the number of bad edges in each part be  $r_1, r_2$  respectively. Then, the *2-min-sum* cost of the corresponding 2-clustering is

$$\frac{(2d)^{1/p}}{2} (|V_1|^2 + |V_2|^2 - n) + (r_1 + r_2)[(2d + 2^p - 2)^{1/p} - (2d)^{1/p}].$$

*Proof.* Let us begin by computing the distance between any two points  $p_u$  and  $p_v$ . Each of the points  $p_u$  and  $p_v$  have  $d$  non-zero entries, since  $G$  is  $d$ -regular. Since we are working in the  $\ell_p$  metric, we remark that

$$\|p_u - p_v\|_p = \left( \sum_{e \in E} |p_u(e) - p_v(e)|^p \right)^{1/p}.$$

## 9:12 On Connections Between $k$ -Coloring and Euclidean $k$ -Means

If there is an edge  $e_0$  from  $u$  to  $v$  in  $G$ , then  $|p_u(e_0) - p_v(e_0)| = 2$  and  $|p_u(e) - p_v(e)| = 1$  for exactly  $2(d-1)$  other edges  $e \in E \setminus \{e_0\}$ . So, the distance between  $p_u$  and  $p_v$  in this case is  $[2(d-1) \cdot 1^p + 2^p]^{1/p} = (2d-2+2^p)^{1/p}$ .

On the other hand, if there is no edge between  $u$  and  $v$ , then  $|p_u(e) - p_v(e)| = 1$  for exactly  $2d$  edges  $e \in E$ . Putting it together, we get:

$$\|p_u - p_v\|_p = \begin{cases} (2d-2+2^p)^{1/p} & \text{if } \{u, v\} \in E, \\ (2d)^{1/p} & \text{otherwise.} \end{cases}$$

The  $2$ -min-sum cost can be computed as follows:

$$\begin{aligned} \sum_{j=1}^2 \sum_{p_u, p_v \in C_j} \|p_u - p_v\|_p &= \sum_{j=1}^2 \left( \binom{|V_j|}{2} - r_j \right) \cdot (2d)^{1/p} + r_j \cdot (2d+2^p-2)^{1/p}, \\ &= \sum_{j=1}^2 \frac{|V_j|(|V_j|-1)}{2} (2d)^{1/p} + r_j((2d+2^p-2)^{1/p} - (2d)^{1/p}), \\ &= \frac{(2d)^{1/p}}{2} (|V_1|^2 + |V_2|^2 - n) + (r_1 + r_2)[(2d+2^p-2)^{1/p} - (2d)^{1/p}]. \quad \triangleleft \end{aligned}$$

### Completeness

In a *YES* instance,  $|V_1| = |V_2| = \frac{n}{2}$  and  $r_1 + r_2 = t$ . So, from Claim 10, the  $2$ -min-sum cost is

$$(2d)^{1/p} \left( \frac{n^2 - 2n}{4} \right) + t[(2d+2^p-2)^{1/p} - (2d)^{1/p}] = \alpha_{n,p,d,t}.$$

### Soundness

In a *NO* instance,  $|V_1| + |V_2| = n$  and  $r_1 + r_2 > t$ . Observe that  $|V_1|^2 + |V_2|^2 \geq n^2/2$ . So the  $2$ -min-sum cost is strictly greater than  $(2d)^{1/p} \left( \frac{n^2 - 2n}{4} \right) + t[(2d+2^p-2)^{1/p} - (2d)^{1/p}] = \alpha_{n,p,d,t}$ .

## 6.2 An $1.7297^n \cdot \text{poly}(n, d)$ runtime Algorithm for 2-min-sum

Instead of giving an algorithm to  $2$ -min-sum problem, we will give a reduction from the problem to the well-known *Max-Cut* problem with linear blowup. Then, we will use the algorithm by Williams [35] that runs in time  $1.7297^n \cdot \text{poly}(n, d)$ , where  $n$  is the number of points.

Let us begin by recalling the well-known NP-Hard problem, the *Max-Cut* problem.

### Max-Cut problem

The input is a weighted graph  $G = (V, E, w)$ , and the output is a partition of the vertices of  $G$  into  $V_1, V_2$  such that the sum of weights of edges with one vertex in  $V_1$  and the other in  $V_2$  is maximized.

► **Lemma 11.** *There is a polynomial-time linear-blowup reduction from 2-min-sum problem to Max-Cut problem.*

**Proof.** Given a  $2$ -min-sum instance  $X \subset (M, d)$ , we will construct a *Max-Cut* instance  $G = (V, E)$  with weight function  $w$ . Let  $n$  be the number of points in  $X$ . For every point  $p \in X$ , we will add a vertex  $v_p$  to  $V$ . We will have an edge between every pair of vertices

$v_p, v_{p'}$  (that is,  $G$  is an  $n$ -clique), and the weight of the edge is equal to distance between the points  $p$  and  $p'$ :  $w(\{v_p, v_{p'}\}) = d(p, p')$ .

*Correctness of the reduction:* For any 2-partitioning of the vertex set  $V = V_1 \dot{\cup} V_2$ , observe that the weight of any edge would either contribute to *Max-Cut* cost or *2-min-sum* cost. To elaborate, the weight of the edge contributes to the *2-min-sum* cost if both the vertices of the edge are in either  $V_1$  or  $V_2$  and to *Max-Cut* cost otherwise. Since the total sum of weights of all the edges in a given instance is constant, *2-min-sum* cost and *Max-Cut* cost sums to a constant. Therefore, maximizing the *Max-Cut* cost is the same task as minimizing the *2-min-sum* cost. ◀

---

## References

- 1 Amir Abboud, Karl Bringmann, Danny Hermelin, and Dvir Shabtay. Seth-based lower bounds for subset sum and bicriteria path. *ACM Transactions on Algorithms (TALG)*, 18(1):1–22, 2022.
- 2 Pranjal Awasthi, Moses Charikar, Ravishankar Krishnaswamy, and Ali Kemal Sinop. The hardness of approximation of euclidean k-means. In Lars Arge and János Pach, editors, *31st International Symposium on Computational Geometry, SoCG 2015, June 22–25, 2015, Eindhoven, The Netherlands*, volume 34 of *LIPICs*, pages 754–767. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2015. doi:10.4230/LIPICs.SOCG.2015.754.
- 3 Richard Beigel and David Eppstein. 3-coloring in time  $O(1.3289^n)$ . *Journal of Algorithms*, 54(2):168–204, 2005.
- 4 P. Berkhin. *A Survey of Clustering Data Mining Techniques*, pages 25–71. Springer Berlin Heidelberg, Berlin, Heidelberg, 2006. doi:10.1007/3-540-28349-8\_2.
- 5 Anup Bhattacharya, Ragesh Jaiswal, and Amit Kumar. Faster algorithms for the constrained k-means problem. *Theory Comput. Syst.*, 62(1):93–115, 2018. doi:10.1007/s00224-017-9820-7.
- 6 Andreas Björklund, Thore Husfeldt, Petteri Kaski, and Mikko Koivisto. Fourier meets möbius: fast subset convolution. In *Proceedings of the thirty-ninth annual ACM symposium on Theory of computing*, pages 67–74, 2007.
- 7 Andreas Björklund, Thore Husfeldt, and Mikko Koivisto. Set partitioning via inclusion-exclusion. *SIAM Journal on Computing*, 39(2):546–563, 2009.
- 8 Vincent Cohen-Addad, Andreas Emil Feldmann, and David Saulpic. Near-linear time approximation schemes for clustering in doubling metrics. In *J. ACM*, volume 68, 2021.
- 9 Vincent Cohen-Addad and Karthik C. S. Inapproximability of clustering in lp metrics. In David Zuckerman, editor, *60th IEEE Annual Symposium on Foundations of Computer Science, FOCS 2019, Baltimore, Maryland, USA, November 9–12, 2019*, pages 519–539. IEEE Computer Society, 2019. doi:10.1109/FOCS.2019.00040.
- 10 Vincent Cohen-Addad, Karthik C. S., and Euiwoong Lee. On approximability of clustering problems without candidate centers. In Dániel Marx, editor, *Proceedings of the 2021 ACM-SIAM Symposium on Discrete Algorithms, SODA 2021, Virtual Conference, January 10 - 13, 2021*, pages 2635–2648. SIAM, 2021. doi:10.1137/1.9781611976465.156.
- 11 Vincent Cohen-Addad, Karthik C. S., and Euiwoong Lee. Johnson coverage hypothesis: Inapproximability of k-means and k-median in  $\ell_p$ -metrics. In Joseph (Seffi) Naor and Niv Buchbinder, editors, *Proceedings of the 2022 ACM-SIAM Symposium on Discrete Algorithms, SODA 2022, Virtual Conference / Alexandria, VA, USA, January 9 - 12, 2022*, pages 1493–1530. SIAM, 2022. doi:10.1137/1.9781611977073.63.
- 12 Marek Cygan, Holger Dell, Daniel Lokshtanov, Dániel Marx, Jesper Nederlof, Yoshio Okamoto, Ramamohan Paturi, Saket Saurabh, and Magnus Wahlström. On problems as hard as CNF-SAT. *ACM Trans. Algorithms*, 12(3):41:1–41:24, 2016. doi:10.1145/2925416.
- 13 David P Dailey. Uniqueness of colorability and colorability of planar 4-regular graphs are np-complete. *Discrete Mathematics*, 30(3):289–293, 1980.

- 14 Andreas Darmann and Janosch Döcker. On a simple hard variant of not-all-equal 3-sat. *Theoretical Computer Science*, 815:147–152, 2020. doi:10.1016/j.tcs.2020.02.010.
- 15 Sanjoy Dasgupta and Yoav Freund. Random projection trees for vector quantization. *IEEE Transactions on Information Theory*, 55(7):3229–3242, 2009.
- 16 W Fernandez De La Vega and Claire Kenyon. A randomized approximation scheme for metric max-cut. *Journal of computer and system sciences*, 63(4):531–541, 2001.
- 17 Uriel Feige. Np-hardness of hypercube 2-segmentation. *arXiv preprint arXiv:1411.0821*, 2014.
- 18 Henry Fleischmann, Kyrylo Karlov, Karthik C. S., Ashwin Padaki, and Stepan Zharkov. Inapproximability of maximum diameter clustering for few clusters. *CoRR*, abs/2312.02097, 2023. doi:10.48550/arXiv.2312.02097.
- 19 Fedor V Fomin, Serge Gaspers, and Saket Saurabh. Improved exact algorithms for counting 3-and 4-colorings. In *Computing and Combinatorics: 13th Annual International Conference, COCOON 2007, Banff, Canada, July 16-19, 2007. Proceedings 13*, pages 65–74. Springer, 2007.
- 20 Fedor V. Fomin, Petr A. Golovach, Tanmay Inamdar, Nidhi Purohit, and Saket Saurabh. Exact exponential algorithms for clustering problems. In Holger Dell and Jesper Nederlof, editors, *17th International Symposium on Parameterized and Exact Computation, IPEC 2022, September 7-9, 2022, Potsdam, Germany*, volume 249 of *LIPICs*, pages 13:1–13:14. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2022. doi:10.4230/LIPICs.IPEC.2022.13.
- 21 Russell Impagliazzo and Ramamohan Paturi. On the complexity of  $k$ -sat. *J. Comput. Syst. Sci.*, 62(2):367–375, 2001. Preliminary version in CCC’99. doi:10.1006/jcss.2000.1727.
- 22 Russell Impagliazzo, Ramamohan Paturi, and Francis Zane. Which problems have strongly exponential complexity? *J. Comput. Syst. Sci.*, 63(4):512–530, 2001. Preliminary version in FOCS’98. doi:10.1006/jcss.2001.1774.
- 23 Mary Inaba, Naoki Katoh, and Hiroshi Imai. Applications of weighted Voronoi diagrams and randomization to variance-based  $k$ -clustering (extended abstract). In *Proceedings of the Tenth Annual Symposium on Computational Geometry, Stony Brook, New York, USA, June 6-8, 1994*, pages 332–339, 1994. doi:10.1145/177424.178042.
- 24 Robert E Jensen. A dynamic programming algorithm for cluster analysis. *Operations research*, 17(6):1034–1057, 1969.
- 25 Robert Krauthgamer and Ohad Trabelsi. The set cover conjecture and subgraph isomorphism with a tree pattern. In Rolf Niedermeier and Christophe Paul, editors, *36th International Symposium on Theoretical Aspects of Computer Science, STACS 2019, March 13-16, 2019, Berlin, Germany*, volume 126 of *LIPICs*, pages 45:1–45:15. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2019. doi:10.4230/LIPICs.STACS.2019.45.
- 26 Amit Kumar, Yogish Sabharwal, and Sandeep Sen. Linear-time approximation schemes for clustering problems in any dimensions. *J. ACM*, 57(2), 2010.
- 27 Michael Lampis. Finer tight bounds for coloring on clique-width. *SIAM Journal on Discrete Mathematics*, 34(3):1538–1558, 2020. doi:10.1137/19M1280326.
- 28 Euiwoong Lee, Melanie Schmidt, and John Wright. Improved and simplified inapproximability for  $k$ -means. *Inf. Process. Lett.*, 120:40–43, 2017. doi:10.1016/j.ipl.2016.11.009.
- 29 Stuart Lloyd. Least squares quantization in pcm. *IEEE transactions on information theory*, 28(2):129–137, 1982.
- 30 Meena Mahajan, Prajakta Nimbhorkar, and Kasturi R. Varadarajan. The planar  $k$ -means problem is NP-hard. *Theor. Comput. Sci.*, 442:13–21, 2012.
- 31 Jaroslav Nešetřil and Svatopluk Poljak. On the complexity of the subgraph problem. *Commentationes Mathematicae Universitatis Carolinae*, 26(2):415–419, 1985.
- 32 Noah Stephens-Davidowitz and Vinod Vaikuntanathan. Seth-hardness of coding problems. In David Zuckerman, editor, *60th IEEE Annual Symposium on Foundations of Computer Science, FOCS 2019, Baltimore, Maryland, USA, November 9-12, 2019*, pages 287–301. IEEE Computer Society, 2019. doi:10.1109/FOCS.2019.00027.

- 33 Ulrike Von Luxburg. A tutorial on spectral clustering. *Statistics and computing*, 17:395–416, 2007.
- 34 R Ryan Williams. *Algorithms and resource requirements for fundamental problems*. PhD thesis, Carnegie Mellon University, 2007.
- 35 Ryan Williams. A new algorithm for optimal 2-constraint satisfaction and its implications. *Theoretical Computer Science*, 348(2-3):357–365, 2005.
- 36 Virginia Vassilevska Williams. Hardness of easy problems: Basing hardness on popular conjectures such as the strong exponential time hypothesis (invited talk). In *10th International Symposium on Parameterized and Exact Computation, IPEC 2015, September 16-18, 2015, Patras, Greece*, pages 17–29, 2015. doi:10.4230/LIPIcs.IPEC.2015.17.
- 37 Virginia Vassilevska Williams. Fine-grained algorithms and complexity (invited talk). In *33rd Symposium on Theoretical Aspects of Computer Science, STACS 2016, February 17-20, 2016, Orléans, France*, pages 3:1–3:1, 2016. doi:10.4230/LIPIcs.STACS.2016.3.
- 38 Virginia Vassilevska Williams. On some fine-grained questions in algorithms and complexity. In *Proc. Int. Cong. of Math.*, volume 3, pages 3431–3472, 2018.
- 39 Virginia Vassilevska Williams, Yinzhan Xu, Zixuan Xu, and Renfei Zhou. New bounds for matrix multiplication: from alpha to omega. In *Proceedings of the 2024 Annual ACM-SIAM Symposium on Discrete Algorithms (SODA)*, pages 3792–3835. SIAM, 2024.
- 40 Xindong Wu, Vipin Kumar, J. Ross Quinlan, Joydeep Ghosh, Qiang Yang, Hiroshi Motoda, Geoffrey J. McLachlan, Angus F. M. Ng, Bing Liu, Philip S. Yu, Zhi-Hua Zhou, Michael S. Steinbach, David J. Hand, and Dan Steinberg. Top 10 algorithms in data mining. *Knowl. Inf. Syst.*, 14(1):1–37, 2008. doi:10.1007/s10115-007-0114-2.
- 41 Or Zamir. Breaking the  $2^n$  barrier for 5-coloring and 6-coloring. In *48th International Colloquium on Automata, Languages, and Programming (ICALP 2021)*. Schloss Dagstuhl – Leibniz-Zentrum für Informatik, 2021.

## A NP-hardness of Balanced Max-Cut

In this section, we prove that the Balanced Max-Cut problem is NP-hard using a particular NP-hard variant of the not-all-equal 3-SAT (abbreviated to “NAE-3-SAT”) problem. For convenience, we write clauses in an instance of 3-SAT as sets of literals, and then consider the instance as a collection of subsets of literals.

### Notations

Given a graph  $G = (V, E)$  and a partition  $V = V_0 \dot{\cup} V_1$ , the *cut* of  $G$  created by  $(V_0, V_1)$  is a subset  $E(V_0, V_1) \subseteq E$  of edges with one end-point in  $V_0$  and the other in  $V_1$ . An edge  $e$  is *good* with respect to a cut  $E(V_0, V_1)$  if  $e \in E(V_0, V_1)$ , and called *bad* otherwise. We denote the number of bad edges by  $\beta(V_0, V_1) := |E| - |E(V_0, V_1)|$ .

Given  $n \in \mathbb{Z}_{\geq 1}$  variables  $x_1, \dots, x_n$ , a *literal* is an element of the set  $X := \{x_{i,a} : i \in [n], a \in \{0, 1\}\}$ . The literal  $x_{i,0}$  will represent the variable  $x_i$ , and  $x_{i,1}$  represents the negation of  $x_i$ , i.e.,  $\bar{x}_i$ .

A *clause* over  $X$  is a subset  $C \subseteq X$  of literals, and a *CNF* over  $X$  is a collection  $\Phi = \{C_1, \dots, C_m\}$  where each  $C_j$  is a clause over  $n$  variables. An *assignment* is a function  $f: X \rightarrow \{0, 1\}$  such that  $f(x_{i,0}) = 1 - f(x_{i,1})$  for each  $i \in [n]$ .

To prove the NP-hardness of Balanced Max-Cut, we give a reduction from Linear 4-Regular NAE-3-SAT, which we define as follows.

### Linear 4-Regular NAE-3-SAT

The input is an integer  $n \in \mathbb{Z}_{\geq 1}$  and a CNF  $\Phi = \{C_1, \dots, C_m\}$  over  $X$  that satisfies

- (3-uniform)  $|C_j| = 3$  for each  $j \in [m]$ ,
- (Linear)  $|C_j \cap C_k| \leq 1$  for all  $j, k \in [m]$  with  $j \neq k$ ,
- (4-regular) For each  $i \in [n]$ , the set  $\{j \in [m] : |C_j \cap \{x_{i,0}, x_{i,1}\}| > 0\}$  has cardinality 4.

The problem outputs *YES* if there exists an assignment  $f: X \rightarrow \{0, 1\}$  with  $f(C_j) = \{0, 1\}$  for each  $j \in [m]$ , and *NO* otherwise.

Essentially,  $f$  as above does not assign every literal in the same clause with the same value; this is the “not-all-equals” part of the problem above.

We call an instance  $\Phi$  of Linear 4-Regular NAE-3-SAT *nae-satisfiable* if there is such an assignment. This problem has been shown to be NP-hard by [14]. We focus now on the main result of this section.

#### A.1 Balanced Max-Cut is NP-hard

Our goal will be to construct a graph  $G = (V, E)$  from an instance  $\Phi$  of Linear 4-Regular NAE-3-SAT by duplicating literals and connecting them by edges in a special way depending on the clauses that contain them.

Fix the number of variables  $n \in \mathbb{Z}_{\geq 1}$  and let  $\Phi := \{C_1, \dots, C_m\}$  be an instance of Linear 4-Regular NAE-3-SAT. We construct a graph  $G = (V, E)$ , depending on  $\Phi$ . Let the vertex set  $V$  of  $G$  be

$$V := X \times [4] = \{(x_{i,a}, k) : x_{i,a} \in X, k \in [4]\},$$

i.e., for every literal in  $X$ ,  $G$  will contain 4 copies of that literal as a vertex.

For each clause  $C_j = \{x_{j_1, a_1}, x_{j_2, a_2}, x_{j_3, a_3}\}$ , introduce an edge between each pair of vertices  $(x_{j_1, a_1}, k), (x_{j_2, a_2}, k), (x_{j_3, a_3}, k) \in V$ , for each  $k \in [4]$ . This constructs four disjoint 3-cycles in  $G$  for  $C_j$ ; denote the  $k$ th one created from  $C_j$  by

$$A_{j,k}^0 := \left\{ \{(x_{j_1, a_1}, k), (x_{j_2, a_2}, k)\}, \{(x_{j_2, a_2}, k), (x_{j_3, a_3}, k)\}, \{(x_{j_3, a_3}, k), (x_{j_1, a_1}, k)\} \right\}.$$

In addition, we also place the same edge relations in  $G$  where we replace  $a_1, a_2, a_3$  with  $1 - a_1, 1 - a_2, 1 - a_3$ , respectively. The edges we have added are those in the set

$$A_{j,k}^1 := \left\{ \{(x_{j_1, 1-a_1}, k), (x_{j_2, 1-a_2}, k)\}, \{(x_{j_2, 1-a_2}, k), (x_{j_3, 1-a_3}, k)\}, \{(x_{j_3, 1-a_3}, k), (x_{j_1, 1-a_1}, k)\} \right\}.$$

Finally, for simplicity, define  $A_{j,k} := A_{j,k}^0 \cup A_{j,k}^1$ , which represents two disjoint triangles in  $G$ .

Next, for each  $i \in [n]$ , insert an undirected edge between  $(x_{i,0}, k) \in V$  and  $(x_{i,1}, \ell) \in V$ , for each  $k, \ell \in [4]$ . This constructs a copy of  $K_{4,4}$  in  $G$  for each  $i \in [n]$ ; denote the edge set of this copy of  $K_{4,4}$  by

$$B_i := \left\{ \{(x_{i,0}, k), (x_{i,1}, \ell)\} : k, \ell \in [4] \right\}.$$

Formally, we’ve constructed the graph  $G = (V, E)$  with edge set

$$E := \bigcup_{j=1}^m \bigcup_{k=1}^4 A_{j,k} \cup \bigcup_{i=1}^n B_i. \quad (3)$$

Intuitively, for each clause  $C_j$ ,  $G$  contains a triangle between the  $k$ th copies of the variables in  $C_j$ , and between their negations. In total, we have 8 disjoint triangles for each clause  $C_j$ . In addition, we connect copies of the variable  $x_{i,0}$  with copies of the variable  $x_{i,1}$  by a copy of  $K_{4,4}$ .



Note that  $G$  is simple (no multiedges) since  $\Phi$  is linear, and  $G$  is 12-regular: each  $(x_{i,a}, k) \in V$  has

$$\deg_G((x_{i,a}, k)) = 12,$$

since  $(x_{i,a}, k)$  is incident to 2 edges for each of the 4 clauses that either  $x_{i,0}$  or  $x_{i,1}$  are in, and  $(x_{i,a}, k)$  is connected to  $(x_{i,1-a}, \ell)$  for  $\ell = 1, \dots, 4$ .

For any cut  $V = V_0 \cup V_1$ , let  $a_{j,k}(V_0, V_1)$  and  $b_i(V_0, V_1)$  be the number of bad edges in  $A_{j,k}, B_i$ , respectively, under the cut  $(V_0, V_1)$ . The union in (3) is actually a disjoint union, so

$$\beta(V_0, V_1) = \left( \sum_{j=1}^m \sum_{k=1}^4 a_{j,k}(V_0, V_1) \right) + \left( \sum_{i=1}^n b_i(V_0, V_1) \right). \quad (4)$$

(For the ease of presentation, we will write  $\sum_{j,k}$  and  $\sum_i$  to represent the sum notations above.)

The next result gives a useful bound for  $\beta$  given the above. Before continuing, observe that the vertices involved in  $A_{j,k}$  and  $B_i$  are

$$V(A_{j,k}) = \{(x_{i,a}, k) : \{x_{i,0}, x_{i,1}\} \cap C_j \neq \emptyset\} \quad \text{and} \quad V(B_i) = \{x_{i,0}, x_{i,1}\} \times [4],$$

correspondingly.

► **Lemma 12.** *For any cut  $(V_0, V_1)$  of  $G$ ,*

$$\beta(V_0, V_1) \geq 8m + 2||V_0| - |V_1||, \quad (5)$$

and, if  $|V_0| = |V_1|$ , equality occurs if and only if  $a_{j,k}(V_0, V_1) = 2$  and  $b_i(V_0, V_1) = 0$  for each  $i, j, k$ .

**Proof.** Any cut of a triangle has either 1 or 3 bad edges, and any cut  $(V'_0, V'_1)$  of  $K_{4,4}$  has at least  $2||V'_0| - |V'_1||$  bad edges (these can be shown through casework). Accordingly, for any cut  $(V_0, V_1)$  of  $G$ ,

$$a_{j,k}(V_0, V_1) \in \{2, 4, 6\} \quad \text{and} \quad b_i(V_0, V_1) \leq 2||V_0^i| - |V_1^i||,$$

where  $V_p^i = V_p \cap V(B_i)$  for  $p = 0, 1$ . Note that  $V_p^1, \dots, V_p^n$  partitions  $V_p$ , so that  $|V_p| = |V_p^1| + \dots + |V_p^n|$ . Hence, from formula (4) for  $\beta(V_0, V_1)$ ,

$$\beta(V_0, V_1) \geq \sum_{j,k} 2 + \sum_i (2||V_0^i| - |V_1^i||) \geq 8m + 2||V_0| - |V_1||.$$

When  $|V_0| = |V_1|$ , equality occurs exactly when  $\beta(V_0, V_1) = 8m$ , which is only possible when each  $a_{j,k}(V_0, V_1) = 2$  and each  $b_i(V_0, V_1) = 0$ . ◀

Now we can prove Theorem 3.

**Proof of Theorem 3.** We prove below the completeness and soundness of the reduction detailed above.

**Completeness.** Suppose  $f: X \rightarrow \{0, 1\}$  nae-satisfies  $\Phi$ . For every  $p \in \{0, 1\}$  we have,

$$V_p = \{(x_{i,a}, k) \in V : f(x_{i,a}) = p\}.$$

By definition of an assignment  $f$ , if  $(x_{i,0}, k) \in V_p$ , then  $(x_{i,1}, k) \in V_{1-p}$ . Hence,  $|V_0| = |V_1| = |V|/2$ . We also obtain that each  $\{(x_{i,0}, k), (x_{i,1}, \ell)\} \in B_i$  is not a bad edge, so  $b_i(V_0, V_1) = 0$  for each  $i \in [n]$ .

Since  $f$  nae-satisfies  $\Phi$ , the image  $f(C_j) = \{0, 1\}$  for each  $j \in [m]$ . Correspondingly, this implies that only one of the three edges in  $A_{j,k}^0$  is a bad edge, and similarly for  $A_{j,k}^1$ . Equivalently,  $a_{j,k}(V_0, V_1) = 2$  for each  $j \in [m], k \in [4]$ . From Lemma 12 for this choice of  $V_0, V_1$ , we have  $\beta(V_0, V_1) = 8m$ .

**9:18 On Connections Between  $k$ -Coloring and Euclidean  $k$ -Means**

**Soundness.** Our proof is by contradiction. Suppose there is some 2-partition  $V := V_0 \dot{\cup} V_1$  such that  $\beta(V_0, V_1) \leq 8m + \frac{t}{|V|} \cdot ||V_0| - |V_1||$ , where  $t = 8m$  and  $|V| = 8n$ , and since  $\Phi$  is 4-Regular NAE-3-SAT formula, we have  $m/n = 4/3$ . By applying Lemma 12 over this partition  $(V_0, V_1)$ , we obtain that  $|V_0| = |V_1|$ . Then, we have that  $\beta(V_0, V_1) = 8m$  and that

$$a_{j,k}(V_0, V_1) = 2 \quad \text{and} \quad b_i(V_0, V_1) = 0,$$

for each  $i \in [n], j \in [m], k \in [4]$ . Since  $b_i(V_0, V_1) = 0$ , it must be the case that, for each  $i \in [n]$  and each  $k, \ell \in [4]$ , the vertices  $(x_{i,0}, k)$  and  $(x_{i,1}, \ell)$  are in different parts of the partition  $V_0 \dot{\cup} V_1 = V$ .

Writing  $X_{i,a} = \{x_{i,a}\} \times [4]$ , observe that the sets  $X_{i,0} := \{x_{i,0}\} \times [4]$  and  $X_{i,1} := \{x_{i,1}\} \times [4]$  are contained in different parts of the partition, that is, either

$$X_{i,0} \subseteq V_0, X_{i,1} \subseteq V_1 \quad \text{or} \quad X_{i,0} \subseteq V_1, X_{i,1} \subseteq V_0.$$

Denote the map  $f: X \rightarrow \{0, 1\}$  by

$$f(x_{i,a}) = \begin{cases} 0 & X_{i,a} \subseteq V_0, \\ 1 & X_{i,a} \subseteq V_1. \end{cases}$$

$f$  is well-defined and  $f(x_{i,0}) = 1 - f(x_{i,1})$ , since  $X_{i,0}, X_{i,1}$  are contained in different parts of the partition.

Finally, if  $a_{j,k} = 2$ , then exactly one of the edges in  $A_{j,k}^0$  is bad, and similarly for  $A_{j,k}^1$ . Correspondingly, this implies that the image set  $f(C_j) = \{0, 1\}$ . Therefore,  $f$  nae-satisfies  $\Phi$ . ◀