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Abstract

The goals of this paper are twofold. First, we formally equate the p-median problem from facility location to the optimal design of a vector quantizer. Second, we use the equivalence to show that the Maranzana Algorithm can be interpreted as a projected Lloyd Algorithm, a fact that improves complexity. Numerical results verify significant improvements in run-time.

Keywords: Facility Location, p-Median Problem, Vector Quantization, Maranzana Algorithm, Lloyd Algorithm.

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1 Introduction

After being introduced by Hakimi [7] in 1965, the p-median problem has become foundational in facility location. In graph theoretical terms, the problem is to find a collection of p positions on a network whose weighted distance to the vertices is as small as possible. The problem is typically presented in operations research as a combinatorial problem like

$$\min \left\{ \sum_{ij} \beta(v_i)\gamma(v_i, v_j)\xi_{ij} : \right.$$
$$\left. \sum_j \xi_{ij} = 1,\ \forall\, i,\ \sum_j \xi_{jj} = p,\ \xi_{jj} \geq \xi_{ij}, \forall\, i, j,\ \xi_{ij} \in \{0, 1\}, \forall\, i, j \right\} \tag{1.1}$$

where $\beta(v_i)$ and $\gamma(v_i, v_j)$ are the node and edge weights and the binary variable ξ_{ij} is such that

$$\xi_{ij} = \begin{cases} 1 & \text{if vertex } v_i \text{ is allocated to vertex } v_j \\ 0 & \text{otherwise,} \end{cases}$$

see for example [1, 16]. This problem is NP-hard in p and the number of vertices, see [11], but is polynomial for fixed p, see [3]. Although the p-median problem is often considered to be discrete, it was at its inception a continuous problem that could be solved by a discrete counterpart like (1.1). We re-visit this context and present a discrete version capable of approximating the original continuous problem.

There are several solution heuristics [14], and one of our goals is to show that under appropriate conditions the Maranzana algorithm can be interpreted as a variant of Lloyd's algorithm from the study of vector quantization (VQ). This observation allows us to reduce the complexity of the algorithm and improve solution time under appropriate conditions. The link between the p-median problem and VQ design rests on formally showing that the two problems are *identical* under appropriate conditions, a result we establish in Section 3.

The following section introduces our notation and model statements, and Section 3 equates the problems. Section 4 discusses complexity and interprets the Maranzana Algorithm as a variant of Lloyds Algorithm. Numerical verification of the complexity analysis is presented in Section 5.

2 Notation and Problem Statements

The p-median problem operates on a (strongly) connected (di)graph $(\mathbb{V}, \mathbb{E})$. We define a *position* on $(\mathbb{V}, \mathbb{E})$ to be either a vertex or a point along an arc, and we write $\mathbb{P} \subseteq (\mathbb{V}, \mathbb{E})$ to mean that $\mathbb{P}$ is a collection of positions on $(\mathbb{V}, \mathbb{E})$. We let $\beta(v)$ be the weight assigned to vertex v and $\gamma(k_i, k_j)$ be the nonnegative value assigned to each ordered pair of positions (k_i, k_j). We do not generally assume that γ is a metric. The continuous version of the p-median problem is to find a collection $\mathbb{P}$ of p positions on $(\mathbb{V}, \mathbb{E})$ that solves

$$\min \left\{ \sum_{k \in \mathbb{P}} \sum_{v \in \mathbb{V}_k} \gamma(k, v)\beta(v) : \mathbb{P} \subseteq (\mathbb{V}, \mathbb{E}),\ |\mathbb{P}| = p \right\}, \tag{2.1}$$

where

$$\mathbb{V}_k = \{v \in \mathbb{V} : \gamma(v, k) \leq \gamma(v, u) \text{ for } u \in \mathbb{P}\}. \tag{2.2}$$

Any collection $\mathbb{P}$ that solves this optimization problem is said to be a collection of *medians*. We are only concerned with a discrete counterpart, and we assume that $\mathbb{P}$ is selected from a set of positions $\mathbb{P}' \subseteq (\mathbb{V}, \mathbb{E})$ with the properties that $\mathbb{V} \subseteq \mathbb{P}'$ and $|\mathbb{P}'| \leq |\mathbb{N}|$, where $\mathbb{N}$ is the set of natural numbers. We refer to this discrete version as *the p-median problem on* $(\mathbb{V}, \mathbb{E})$ *restricted to* $\mathbb{P}'$ *with respect to* (γ, β), which is

$$\min \left\{ \sum_{k \in \mathbb{P}} \sum_{v \in \mathbb{V}_k} \gamma(v, k)\beta(v) : \mathbb{P} \subseteq \mathbb{P}',\ |\mathbb{P}| = p \right\}. \tag{2.3}$$

The sets $\mathbb{V}_k$ are not necessarily unique, and if v is a candidate for multiple $\mathbb{V}_k$'s, then v is placed uniquely in the one with smallest index k. This condition is allowed due to the assumption that $|\mathbb{P}'| \leq \mathbb{N}$ and, as shown the next section, is important in our ability of equating the problem to VQ design. As a note on other usages of the term median, the *median subgraph of a graph* is the induced subgraph of all 1-medians in which $\mathbb{P}' = \mathbb{V}$ [5].

Vector quantization is a process that codes continuous or discrete signals subject to a fidelity criterion and is often used to compress images or other data. A *vector quantizer*, or simply a quantizer, is a mapping $\mathcal{Q}$ from an input set of vectors $\mathbb{V}$ onto a p element subset $\mathcal{C}$ of $\mathbb{V}$ —i.e. $\mathcal{Q} : \mathbb{V} \overset{\text{onto}}{\rightarrow} \mathcal{C} \subseteq \mathbb{V}$, where $|\mathcal{C}| = p$. The image set $\mathcal{C}$ is called the *codebook* and its elements are called *codevectors* or *codewords*. A quantizer partitions $\mathbb{V}$ into p distinct regions called *cells*, which are defined for every $\hat{v} \in \mathcal{C}$ by

$$\mathbb{V}_{\hat{v}} = \{v \in \mathbb{V} \mid \mathcal{Q}(v) = \hat{v}\}.$$

Quantizers are typically separated into two processes, known as the *encoder*, $\mathcal{E}$, and the *decoder*, $\mathcal{D}$. The encoder assigns an input vector to a partition cell, and hence, $\mathcal{E} : \mathbb{V} \rightarrow \{1, 2, \ldots, p\}$. The decoder selects a vector from each cell to serve as that cell's codevector. So, $\mathcal{D} : \{1, 2, \ldots, p\} \rightarrow \mathcal{C}$ and $Q(v) = \mathcal{D}(\mathcal{E}(v))$. A common example is found in analog to digital conversion, where a continuous analog signal is quantized into a finite collection of digital signals. For example, a human's auditory range is between 20 and 20,000 Hz. If the digital storage medium only distinguishes between p different signals, a simple encoder would map the interval $[20 + 19980(i -$

$1)/p\,,\, 20 + 19980i/p]$ to the integer i, for $i = 1, 2, \ldots, p$. A simple decoder would map i to the midpoint of the interval, $i \mapsto 20 + 19980(i - 1/2)/p$. Such a quantizer mimics the rounding process. A discrete example is to let $\mathbb{V}$ be a finite set of points on a city map. Consider an encoder that maps these locations into school districts, each represented by a district number. The decoder then maps the index number of a particular district to the location for that district's school. In this work we only consider discrete quantizers, and hence $|\mathbb{V}| \le |\mathbb{N}|$.

A quantizer's performance is evaluated in terms of *distortion*, which relies on two pieces of information. The first of these is a real value that represents the similarity between any two input vectors, and allowing $\mathbb{R}_+$ to be the set of nonnegative real values, we let $\rho : \mathbb{V} \times \mathbb{V} \to \mathbb{R}_+$ map the ordered pair (v_i, v_j) to the nonnegative similarity $\rho(v_i, v_j)$, which measures how similar v_i is to v_j. As with γ, we do not generally assume that ρ is a metric. That said, two common measures are $\rho(v_i, v_j) = \|v_i - v_j\|^2$ and $\rho(v_i, v_j) = \|v_i - v_j\|$, and within information theory these problems are commonly referred to as the k-means and k-median problems, respectively [1] [10]. The second piece of information is the probability of observing an input vector, and we assume that $\alpha(v)$ is the probability of observing v.

A quantizer's expected distortion is

$$D_{\mathcal{Q}} = E\rho(v, \mathcal{Q}(v)) = \sum_i \rho(v_i, \mathcal{Q}(v_i))\alpha(v_i),$$

where i indexes the elements of $\mathbb{V}$, and the design problem is to find a quantizer that minimizes distortion. The feasible region for the design process is the collection of p element subsets of $\mathbb{V}$, making the size of the feasible region $\binom{|\mathbb{V}|}{p}$ if $|\mathbb{V}| < |\mathbb{N}|$ or $|\mathbb{N}|$ if $|\mathbb{V}| = |\mathbb{N}|$. For any particular p element subset of $\mathbb{V}$, say $\mathbb{W}$, the partition cell for each $w \in \mathbb{W}$ that minimize the distortion is

$$\mathbb{V}_w = \{v \in \mathbb{V} : \rho(v, w) \le \rho(v, u) \ \text{ for } \ u \in \mathbb{W}\}. \tag{2.4}$$

As with the definition of $\mathbb{V}_k$, the set $\mathbb{V}_w$ is not necessarily unique because some of the elements of $\mathbb{V}$ may be equally similar to several elements of $\mathbb{W}$, and we again assign such elements to the $\mathbb{V}_w$ with the smallest indexed w. With this notation, the *p-element VQ design problem on $\mathbb{V}$ with respect to* (ρ, α) is

$$\min \left\{ \sum_{w \in \mathbb{W}} \sum_{v \in \mathbb{V}_w} \rho(v, w)\alpha(v) : \mathbb{W} \subseteq \mathbb{V},\ |\mathbb{W}| = p \right\}. \tag{2.5}$$

Some historical notes are warranted to position our work within the current research environment. Hakimi's original work [6, 7] assumed a (strongly) connected

[1]The similarity between the titles of the p-median from facility location and the k-median problem from information theory is awkward, but the problems are generally different. Each problem has a history in its host discipline. Part of this work provides conditions under which the problems are the same.

and non-negatively weighted (di)graph for which $\gamma(k_i, k_j)$ was the length of the shortest path from position k_i to position k_j. Under the additive condition that $\gamma(v_i, v_j) = \gamma(v_i, k) + \gamma(k, v_j)$ for any position k on edge (v_i, v_j), Hakimi established the following result.

Theorem 2.1 (Hakimi [6, 7]) *If G is a connected (di)graph with nonnegative vertex and edge weights, then there is a collection of p vertices that are also medians.*

This result's impact lies in the fact that the solution set to the original, continuous p-median problem contains the solutions to a combinatorial problem like (1.1). However, the p-median problem is often stated as a combinatorial problem without regards to it's continuous underpinning. At issue is the fact that Hakimi's proof assumed an additive property that may or may not be appropriate for an application, and hence, the combinatorial problem might fail to solve the intended continuous problem. In fact, vertex restrictions of similar continuous problems like the p-center problem are not generally possible, see [1] and its citations. Although our analysis in the following section was motivated by improving the efficiency of the Maranzana heuristic to solve the combinatorial problem, it also, in some way, extends Hakimi's result since it removes the assumed additive property. The extension is not exact since the discrete version of the problem in (2.3) can only approximate the continuous problem since $\mathbb{P}'$ can at best be a dense subset of the (di)graph.

3 Problem Equivalence

A standard concept of 'equivalent' mathematical programs is not widely accepted within the optimization community. We use an equivalence relation that requires problems to be invertible transformations of each other. To be precise, we say that the problems

$$P1 : \min\{f(x) : x \in X\} \quad \text{and} \quad P2 : \min\{g(y) : y \in Y\} \tag{3.1}$$

are *identical* under h if there is a bijection $h : X \to Y$ such that $f = g \circ h$. This sense of equivalence is strong and essentially states that we have simply re-labeled the elements of the feasible region in a way that maintains the objective value. Some immediate observations are

1. if $P1$ is identical to $P2$ under h, then

$$h(\text{argmin}\{f(x) : x \in X\}) = \text{argmin}\{g(y) : y \in Y\}) \text{ and}$$

2. the equivalence class of $P1$, denoted $[f, X]$, is

$$[f, X] = \{(g, Y) : h(X) = Y \;\text{ and }\; f = g \circ h, \;\text{ for some bijection }\; h : X \to Y\}.$$

The problem statements in (2.3) and (2.5) were modeled to highlight their similarity. Indeed, we purposefully used $\mathbb{V}$ to denote both the vertex set of the digraph and the set of vectors to be quantized to highlight this connection. However, those studying VQ design typically address a stochastic problem, and those interested in the p-median problem are generally concerned with a deterministic, combinatorial problem. In the end, the problems are identical, a statement made rigorous in Theorem 3.1. Others have noticed a connection; for example, a VQ application in [9] is said to be "equivalent to a directional p-median problem in multiple dimensions." However, to the authors' knowledge the literature has lacked a rigorous argument detailing the relationship between the two. Although the proof is straightforward, the theorem's conditions and the examples that follow show that the problems are generally not the same.

Theorem 3.1 *Let $\mathbb{P}'$ be a discrete collection of positions on the (strongly) connected (di)graph $(\mathbb{V}, \mathbb{E})$. Let $\beta : \mathbb{P}' \to \mathbb{R}_+$ satisfy $\sum_{v \in \mathbb{V}} \beta(v) = 1$ and $\beta(v) = 0$ if $v \in \mathbb{P}' \backslash \mathbb{V}$. Further assume that γ is any map from $\mathbb{P} \times \mathbb{P}$ into $\mathbb{R}_+$. Then the following problems are identical.*

1. *The p-element VQ design problem on $\mathbb{P}'$ with respect to (γ, β),*

2. *The p-median problem on the complete digraph $(\mathbb{P}', \mathbb{P}' \times \mathbb{P}')$ restricted to $\mathbb{P}'$ with respect to (γ, β), and*

3. *The p-median problem on $(\mathbb{V}, \mathbb{E})$ restricted to $\mathbb{P}'$ with respect to (γ, β).*

Proof: From (2.5) and (2.3) we see that problems 1 and 2 are respectively

$$\min \left\{ \sum_{w \in \mathbb{W}} \sum_{v \in \mathbb{V}_w} \gamma(v, w)\beta(v) : \mathbb{W} \subseteq \mathbb{P}', \ |\mathbb{W}| = p \right\} \tag{3.2}$$

and

$$\min \left\{ \sum_{k \in \mathbb{P}} \sum_{v \in \mathbb{V}_k} \gamma(v, k)\beta(v) : \mathbb{P} \subseteq \mathbb{P}', \ |\mathbb{P}| = p \right\}. \tag{3.3}$$

We define the bijection from the feasible region of (3.2) onto (3.3) by

$$h(\mathbb{W}) = \mathbb{P} \ \text{ if and only if } \ \mathbb{W} = \mathbb{P}.$$

This is nothing more than the identity map on the collection of p-element subsets of $\mathbb{P}'$. So for any feasible $\mathbb{W}$ in (3.2) we have $h(\mathbb{W}) = \mathbb{P}$ is feasible in (3.3). This allows w and k in the outer summations to be the same, and we subsequently have from (2.2) and (2.4) that the index sets for the inner summations coincide. We conclude the problems are identical.

Consider problems 2 and 3, which have the same feasible region. This allows us to use the identity map $\hat{h}(\mathbb{P}) = \mathbb{P}$. Unfortunately, the index sets of the inner summations do not agree since the vertex set for problem 3 is $\mathbb{V}$ and the vertex set for problem 2 is $\mathbb{P}'$. This means the index set of the inner summation for problem 3 is

$$\mathbb{V}_k = \{v \in \mathbb{V} : \gamma(v,k) \leq \gamma(v,u) \text{ for } u \in \mathbb{P}\},$$

while the index set for problem 2 is

$$\hat{\mathbb{V}}_k = \{v \in \mathbb{P}' : \gamma(v,k) \leq \gamma(v,u) \text{ for } u \in \mathbb{P}\}.$$

However, since $\beta(v) = 0$ for $v \in \mathbb{P}' \backslash \mathbb{V}$, we have for any $k \in \mathbb{P}'$ that

$$\sum_{v \in \mathbb{V}_p} \gamma(v,k)\beta(v) = \sum_{v \in \hat{\mathbb{V}}_p} \gamma(v,k)\beta(v),$$

and hence, the objective values agree under $\hat{h}$. We conclude that problems 2 and 3 are identical. The fact that problems 1 and 3 are identical follows by considering the composition of h and $\hat{h}$, which is again the identity map. ■

We mention that one choice for $\mathbb{P}'$ is $\mathbb{V}$, which supports problems statements like (1.1). We further mention that the manner in which (2.3) and (2.5) are stated is important to the theorem's conclusion. Typically, both problems are stated in terms of selecting a subset of vectors or vertices, referred to as *selection*, and assigning the vectors or vertices to the selected elements, referred to as *assignment*. The optimization problems in (2.3) and (2.5) do not consider assignment in their descriptions of the feasible regions. Instead, both feasible regions are the p-element subsets of the vertices or vectors and the assignments are described by the index set of the inner summation. This is allowed because each p-element subset defines a unique optimal assignment as defined in (2.2) and (2.4). The fact that some elements may have equal similarity means there may be numerous alternative assignments. However, the discrete assumption implies the vertices of the digraph and the vectors to be quantized are at most countable. This is crucial to the proof since it allows us to define a unique assignment for each feasible subset with the least index rule.

To highlight the importance of the least index rule, let $(\mathbb{V}, \mathbb{E})$ be the digraph in Figure 1 for problem 3 in Theorem 3.1. The corresponding complete digraph for problem 2 is in Figure 2 (arrows are not shown). The problem on $(\mathbb{V}, \mathbb{E})$ only assigns positions k_1, k_3 and k_4 —i.e. the vertices in $\mathbb{V}$, whereas the problem on $(\mathbb{P}', \mathbb{P}' \times \mathbb{P}')$ assigns $k_1, k_2, \ldots, k_6$ —i.e. the elements of $\mathbb{P}'$. Suppose we are solving the 2-median problem and that γ and β are such that

- $\{k_1, k_4\}$ is the unique solution (notice this is for both problems), and
- for the problem on $(\mathbb{V}, \mathbb{E})$ we have $\mathbb{V}_{k_1} = \{k_1\}$ and $\mathbb{V}_{k_4} = \{k_3, k_4\}$.

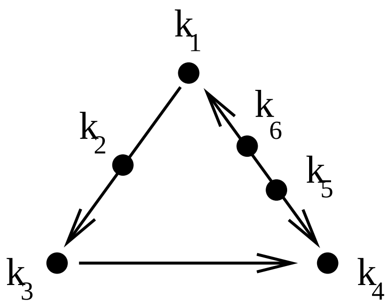

Figure 1: A strongly connected digraph with 3 added positions to select medians from.

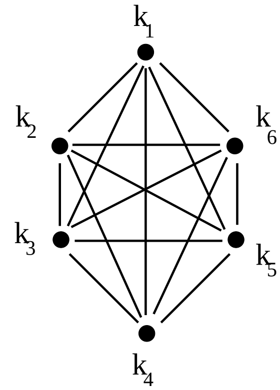

Figure 2: The corresponding complete graph of the digraph in Figure 1, all edges are bi-directional arcs.

Considering the problem for $(\mathbb{P}', \mathbb{P}' \times \mathbb{P}')$, we see k_2, k_5 and k_6 need to be added to either $\mathbb{V}_{k_1}$ or $\mathbb{V}_{k_4}$, and our construction says they are assigned to k_1 or k_4 depending on to which they are more similar. However, we could have $\gamma(k_i, k_j) = 0$ for $i = 2, 5, 6$ and $j = 1, 3, 5$, meaning k_2, k_5 and k_6 are equally similar to each of the elements in $\mathbb{V}$. Our construction dictates that k_2, k_5 and k_6 are each assigned to the median with the lowest index, and using the notation from the proof of Theorem 3.1, we have $\hat{\mathbb{V}}_{k_1} = \{k_1, k_2, k_5, k_6\}$ and $\hat{\mathbb{V}}_{k_4} = \{k_3, k_4\}$, which is a unique assignment. If the least index rule was removed, then there would have been 8 possible ways to add k_2, k_5 and k_6 to $\mathbb{V}_{k_1}$ and $\mathbb{V}_{k_4}$. If the feasible regions had been stated in terms of both selection and assignment without regard to some tie braking rule for the assignment decision, then this would have violated the necessity of the argument minimums having the same cardinality, and hence, the problems would not have been identical. From this perspective the simple proof of Theorem 3.1 is a byproduct of modeling, as the same sense of equality would not have been possible with a combinatorial statement like (1.1). It is likely that one could address the problem in the continuum by invoking the axiom of choice.

Theorem 3.1 has two substantive corollaries.

Corollary 3.2 *Every discrete p-element VQ design problem corresponds to a discrete p-median problem on a complete digraph restricted to the vertices.*

This follows immediately from the fact that problems 1 and 2 in Theorem 3.1 are identical. The idea is to start with a p-element VQ design problem and simply construct the complete digraph whose vertices are the vectors in the quantization problem. This

p-median problem is restricted to the vertices, which allows the similarity measure ρ in the quantization problem to fulfill the role of γ in the p-median problem. Similarly, the vertex weights in the k-median problem are the probability measures in the quantization problem.

The second corollary is similar to Hakimi's original result since it states that we only need to consider vertex solutions of an associated graph.

Corollary 3.3 *For every discrete p-median problem there is an alternative p-median problem in which only collections of vertices need to be considered. Moreover, this alternative p-median problem corresponds to a p-element VQ design problem.*

Similar to the previous corollary, this statement follows immediately from the fact that problems 1, 2 and 3 in Theorem 3.1 are identical. However, a graph description is warranted. Consider the p-median problem on $(\mathbb{V}, \mathbb{E})$ restricted to $\mathbb{P}'$ with respect to (γ, β). Recall that γ is defined for every pair in $\mathbb{P}' \times \mathbb{P}'$. This means we can consider the complete digraph $(\mathbb{P}', \mathbb{P}' \times \mathbb{P}')$ with edge weights defined by γ. This complete digraph does not have node values for the vertices in $\mathbb{P}' \backslash \mathbb{V}$, and we extend the definition of β to $\hat{\beta}$ so that $\hat{\beta}(k) = \beta(k)$ if $k \in \mathbb{V}$ and $\hat{\beta}(k) = 0$ if $k \in \mathbb{P}' \backslash \mathbb{V}$. This extension satisfies the conditions of Theorem 3.1, and hence, we only need to consider collections of vertices of the complete digraph to solve the discrete problem on $(\mathbb{V}, \mathbb{E})$ restricted to $\mathbb{P}'$. This argument is similar to Hakimi's original proof since he constructs a complete graph with the shortest-path metric. As mentioned earlier Hakimi's proof requires an additive property along arcs, which is reasonable in some settings but inappropriate in others. Our approach does not require this additive property.

4 Solution Techniques & Complexity

Kariv and Hakimi [11] showed that the problem of finding a p-median on a connected digraph is NP-hard in p and $|\mathbb{V}|$. Polynomial algorithms exist, however, if p is fixed [3].

Although our discrete version of the p-median problem is different than Hakimi's original statement, the following result states the related conclusion that the discrete p-median problem on $(\mathbb{V}, \mathbb{E})$ restricted to $\mathbb{P}'$ with respect to (γ, β) is polynomial as long as p is fixed.

Theorem 4.1 *Assuming $|\mathbb{P}'|$ is finite, we have the worst-case complexity of the discrete k-median problem on $G = (\mathbb{V}, \mathbb{E})$ restricted to $\mathbb{P}'$ with respect to (γ, β) is $O(|\mathbb{V}||\mathbb{P}'|^{p+1})$.*

Proof: The size of the feasible region is $\binom{|\mathbb{P}'|}{p} = O(|\mathbb{P}'|^p)$. We need to compare each element of a feasible $\mathbb{P}$ to the elements of $\mathbb{V}$ to form $\mathbb{V}_k$, which is $O(|\mathbb{V}||\mathbb{P}'|)$. So, starting with $(\mathbb{V}, \mathbb{E})$ and $\mathbb{P}'$, we require no more than $O(|\mathbb{V}||\mathbb{P}'|^{p+1})$ iterations to define (2.3). The addition in the objective function requires no more than $O(p|\mathbb{V}|)$ multiplications. Hence, the total computation requires no worse than $O(|\mathbb{V}||\mathbb{P}'|^{p+1} + p|\mathbb{V}|) = O(|\mathbb{V}||\mathbb{P}'|^{p+1})$ iterations. ■

Notice that since $\mathbb{V} \subseteq \mathbb{P}'$, we also have the complexity is no worse than $O(|\mathbb{P}'|^{p+2})$, which is less impressive for the p-median problem but appropriate for VQ design since $\mathbb{V} = \mathbb{P}'$. This leads to the following corollary.

Corollary 4.2 *The worst-case complexity of the p-element VQ design problem on $\mathbb{P}'$ with respect to (γ, β) is $O(|\mathbb{P}'|^{p+2})$.*

Proof: From Theorem 3.1 we have that if $\mathbb{V} = \mathbb{P}'$, then the problems are identical, which establishes the result. ■

Polynomial time does not mean heuristics are unimportant, and the computational demand in many applications exceeds modern capabilities. Numerous heuristics have been proposed for both problems, and a benefit of Theorem 3.1 is that it allows us to model a situation as either median location or VQ design, depending on which is cognitively simpler, but heuristically solve the problem with techniques from either realm. The rest of this section compares some of the common heuristics for both problems, and we show that under certain conditions the Maranzana algorithm for the p-median problem can be interpreted as a discrete version of Lloyd's algorithm for VQ design. We call the blended variant the *discrete Lloyd algorithm*.

The Maranzana algorithm for the p-median problem was first proposed in 1964 [13], and Lloyd's algorithm for VQ design was originally proposed in an unpublished technical report in 1957 and later published in 1982 [12] (this issue of IEEE Transactions on Information Theory is particularly good for operation researchers interested in the k-means and k-median problems). Both techniques iterate between the assignment and selection parts of the problem in a way that improves the objective function. In terms of (2.3) and (2.5), both algorithms begin with an initial feasible element, $\mathbb{P}$ and $\mathbb{W}$. The assignment part is the construction of the inner summations' index sets, $\mathbb{V}_k$ for $k \in \mathbb{P}$ and $\mathbb{V}_w$ for $w \in \mathbb{W}$. The selection part of the problem is to update $\mathbb{W}$ and $\mathbb{P}$ by respectively calculating for each $k \in \mathbb{P}$ and $w \in \mathbb{W}$

$$\text{argmin}\left\{\sum_{v \in \mathbb{V}_k} \gamma(v,u)\beta(v) : u \in \mathbb{V}_k\right\} \tag{4.1}$$

and

$$\text{argmin}\left\{\sum_{v \in \mathbb{V}_w} \rho(v,u)\alpha(v) : u \in \mathbb{V}_w\right\}. \tag{4.2}$$

An element from each argument minimum is selected to form the new feasible sets, say $\hat{\mathbb{W}}$ and $\hat{\mathbb{P}}$, which replace $\mathbb{W}$ and $\mathbb{P}$. The process continues until $\hat{\mathbb{W}} = \mathbb{W}$ and $\hat{\mathbb{P}} = \mathbb{P}$. The objective function is non-increasing with every new $\hat{\mathbb{W}}$ and $\hat{\mathbb{P}}$, see [4] and [13].

The conditions of Theorem 3.1 together with the assumption that (4.1) and (4.2) contain a unique element guarantee the two algorithms produce the same iterates if applied to the same problem and initialized in the same way. However, the Lloyd and Maranzana algorithms differ in how they calculate an element of (4.1) and (4.2).

The k-means version of VQ design assumes $\rho(v_i, v_j) = \|v_i - v_j\|^2$, and in the continuum this means the center-of-mass of each cell minimizes the the cell's expected distortion -i.e.

$$\left\{ \frac{\sum_{v \in \mathbb{V}_w} \alpha(v) v}{\sum_{v \in \mathbb{V}_w} \alpha(v)} \right\} = \operatorname{argmin} \left\{ \sum_{v \in \mathbb{V}_w} \|x - v\|^2 \alpha(v) : x \in \mathbb{R}^n \right\}. \tag{4.3}$$

Calculating the center-of-mass requires the product $\alpha(v)v$ to be well defined, which is true if $\mathbb{V}$ is a vector space built on a scalar field containing the range of α. Traditional VQ problems are cast in the continuum with $\mathbb{V} = \mathbb{R}^n$ and $\alpha(\mathbb{V}) \subseteq \mathbb{R}$, and hence the computation is well-defined. Our discrete version allows the dense approximation $\mathbb{V} = \mathbb{Q}^n$ with $\alpha(\mathbb{V}) \subseteq \mathbb{Q}$, which reduces the problem to rational arithmetic.

A concern in the discrete setting is that we are not guaranteed $\mathbb{V}$ contains the center-of-mass even if the arithmetic is well defined. This is not an issue if $\mathbb{V} = \mathbb{Q}$ but is a problem in the common situation of $\mathbb{V}$ being finite. However, if we assume that $\alpha(v)$ is constant, which is the same as assuming the elements of $\mathbb{V}$ are uniformly distributed, then we show that the projection of the center-of-mass onto $\mathbb{V}_w$ is an element of (4.2). We let $\text{proj}_{\mathbb{V}_w}(v)$ be the nearest element of $\mathbb{V}_w$ to v, with ties being decided by the least index rule, and show that this element is in the desired argument minimum. Similar ideas are found in [2].

Theorem 4.3 *Assume $\mathbb{W} \subseteq \mathbb{V}$, $|\mathbb{V}| < \infty$, $\rho(v_i, v_j) = \|v_i - v_j\|^2$ and $\alpha(v)$ is constant. Then, for each $w \in \mathbb{W}$ we have*

$$\mathit{proj}_{\mathbb{V}_w} \left(\frac{1}{|\mathbb{V}_w|} \sum_{u \in \mathbb{V}_w} u \right) \in \operatorname{argmin} \left\{ \sum_{v \in \mathbb{V}_w} \|u - v\|^2 : u \in \mathbb{V}_w \right\}.$$

Proof: Let $w \in \mathbb{W}$ and $M = (1/|\mathbb{V}_w|) \sum_{w \in \mathbb{V}_w} w$. Since $\alpha(v)$ is constant, we have from (4.3) that

$$\begin{aligned} & \min \left\{ \sum_{v \in \mathbb{V}_w} \|u - v\|^2 : u \in \mathbb{V}_w \right\} \\ = \; & \min_{k \geq 0} \left\{ \sum_{v \in \mathbb{V}_w} \|M - v\|^2 + k : \right. \\ & \qquad \left. \mathbb{V}_w \cap \left\{ x \in \mathbb{R}^n : \sum_{v \in \mathbb{V}_w} \|x - v\|^2 \leq \sum_{v \in \mathbb{V}_w} \|M - v\|^2 + k \right\} \neq \emptyset \right\}. \end{aligned}$$

Since

$$\begin{aligned}
&\left\{x \in \mathbb{R}^n : \sum_{v \in \mathbb{V}_w} \|x - v\|^2 \le \sum_{v \in \mathbb{V}_w} \|M - v\|^2 + k\right\} \\
&= \left\{x \in \mathbb{R}^n : \sum_{v \in \mathbb{V}_w} \big((x-v)^T(x-v) - (M-v)^T(M-v)\big) \le k\right\} \\
&= \left\{x \in \mathbb{R}^n : \sum_{v \in \mathbb{V}_w} \big(x^Tx - 2x^Tv - M^TM + 2M^Tv\big) \le k\right\} \\
&= \left\{x \in \mathbb{R}^n : \frac{1}{|\mathbb{V}_w|} \sum_{v \in \mathbb{V}_w} x^Tx - 2x^T \left(\frac{1}{|\mathbb{V}_w|} \sum_{v \in \mathbb{V}_w} v\right) - \right. \\
&\qquad \left. \frac{1}{|\mathbb{V}_w|} \sum_{v \in \mathbb{V}_w} M^TM + 2M^T \left(\frac{1}{|\mathbb{V}_w|} \sum_{v \in \mathbb{V}_w} v\right) \le \frac{k}{|\mathbb{V}_w|}\right\} \\
&= \left\{x \in \mathbb{R}^n : x^Tx - 2x^TM - M^TM + 2M^TM \le k/|\mathbb{V}_w|\right\} \\
&= \left\{x \in \mathbb{R}^n : x^Tx - 2x^TM + M^TM \le k/|\mathbb{V}_w|\right\} \\
&= \left\{x \in \mathbb{R}^n : \|x - M\|^2 \le k/|\mathbb{V}_w|\right\} \\
&= \left\{x \in \mathbb{R}^n : \|x - M\| \le \sqrt{k/|\mathbb{V}_w|}\right\},
\end{aligned}$$

the optimal value of

$$\min \left\{\sum_{v \in \mathbb{V}_w} \|u - v\|^2 : u \in \mathbb{V}_w\right\} \tag{4.4}$$

is $\sum_{v \in \mathbb{V}_w} \|M - v\|^2 + k$, where k is the smallest value such that

$$\left\{x \in \mathbb{R}^n : \|x - M\| \le \sqrt{k/|\mathbb{V}_w|}\right\} \cap \mathbb{V}_w \ne \emptyset.$$

Since the left-hand set is a ball around M of radius $\sqrt{k/|\mathbb{V}_w|}$, we have from the definition of $\mathrm{proj}_{\mathbb{V}_w}(M)$ that the smallest value $\sqrt{k/|\mathbb{V}_w|}$ with this property is $\|(M - \mathrm{proj}_{\mathbb{V}_w}(M))\|$, which shows that $\mathrm{proj}_{\mathbb{V}_w}(M)$ solves (4.4). ■

From this result we have that in the finite case an element of (4.2) can be calculated by projecting the center-of-mass onto $\mathbb{V}_w$, provided that $\alpha(v)$ is constant. Both calculating the center-of-mass and projecting it onto $\mathbb{V}_w$ are $O(|\mathbb{V}|)$, which means the complexity of calculating $\hat{\mathbb{W}}$ is $O(k|\mathbb{V}|)$. In contrast the Maranzana heuristic doesn't assume any geometric structure of γ and β, and hence, the construction of $\hat{\mathbb{P}}$ requires pairwise comparisons within each $\mathbb{V}_p$, which is $O(k|\mathbb{V}|^2)$. So in the finite case when α is constant and ρ is squared error, Lloyd's approach of using the center-of-mass has lower complexity. In the rest of the paper we assume that α is constant, ρ is squared error, $\beta = \alpha$, $\gamma = \rho$, and $\mathbb{P}' = \mathbb{V}$ so that (4.1) and (4.2) are the same. In this case we can calculate an element of (4.1) with either the pairwise comparisons of the original Maranzana algorithm or by projecting the the center-of-mass of each $\mathbb{V}_k$ onto $\mathbb{V}_k$. We refer to the latter algorithm as the discrete Lloyd algorithm (DLA). A least indexing rule is used to ensure that the same element from (4.1) is selected independent of which technique is used.

A point of note is that Lloyd's approach only aligns with the Maranzana algorithm because the projection is onto $\mathbb{V}_k$. If the projection had instead been onto $\mathbb{V}$, which would have been an alternative discrete counterpart, then the two heuristics would not generally produce the same sequence of iterates even if (4.1) and (4.2) were singletons. However, the examples exhibiting the difference are contrived. To compare the two we ran 1000 instances each in which $p = 5$, $|\mathbb{V}|$ was either 250, 500, or 1000, and the elements of $\mathbb{V}$ were uniformly distributed over $[0,1]^2$. In all 3000 instances the projections onto $\mathbb{V}_k$ and $\mathbb{V}$ were the same, but the technique projecting onto $\mathbb{V}$ increased our run time by a factor of 3.2. For this reason, we only consider projections onto $\mathbb{V}_k$.

5 Numerical Experiment

In this section we numerically compare the performance of several solution techniques. In addition to the Maranzana algorithm and DLA, we include comparisons with vertex substitution (VS) [17, 18, 19], which was originally developed in 1968 by Teitz and Bart [20]. Each iteration of VS decides whether or not to swap a position in $\mathbb{P}$ with a position not in $\mathbb{P}$. Variations differ in how they select the elements to swap. In 1983, Whitaker [21] developed an implementation known as fast interchange, which was later implemented in the Variable Neighborhood Search method of Hansen and Mladenović [8]. Both of these implementations begin by searching through $\mathbb{V}\backslash\mathbb{P}$ and testing whether swapping with an element of $\mathbb{P}$ would reduce the objective function. Whitaker's method performs the swap with the first profitable position found, whereas the Hansen and Mladenović implementation tests all possible swaps and performs the one most profitable. Interested readers are directed to [8] and [15] for complete descriptions.

We assume all examples are complete digraphs for which $\mathbb{P}' = \mathbb{V} \subseteq \mathbb{R}^3$, $|\mathbb{V}| < \infty$, $\beta(v) = 1$ and $\gamma(v_1, v_2) = \|v_1 - v_2\|^2$. Problems are identified by the tuple $(|\mathbb{V}|, p)$, so $(1000, 15)$ is an instance with 1000 nodes and 15 medians, We randomly generated $\mathbb{V}$ with MATLAB 7.0 and considered all instances $(|\mathbb{V}|, p)$ in

$$\{100, 250, 500, 1000, 1200, 1500, 2000\} \times \{5, 10, 15, 20, 30\},$$

producing 35 different problems in the unit hypercube of $\mathbb{R}^3$. For each problem we randomly generated 30 different p-element subsets of $\mathbb{V}$ to use as starting points for

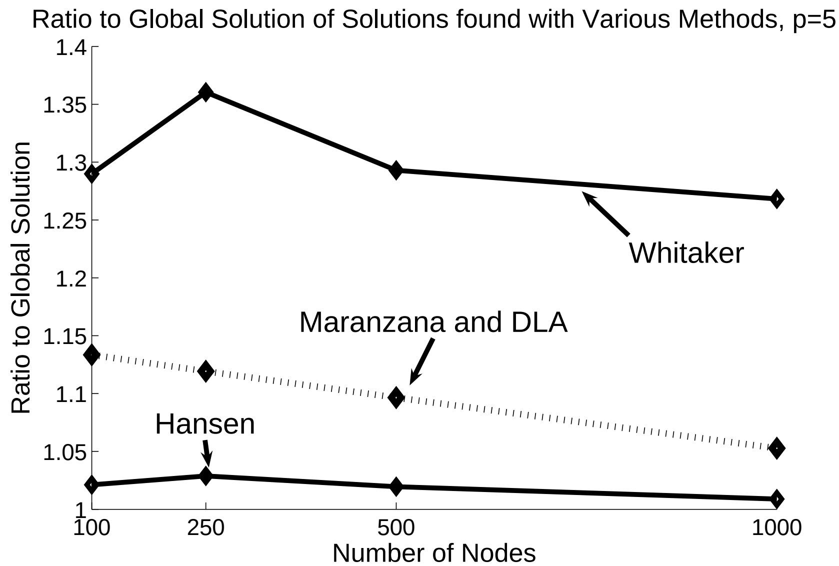

Figure 3: The average objective value as a ratio of the global solution versus $|\mathbb{V}|$ with $p = 5$. Each technique appears to improve its solution quality as $|\mathbb{V}|$ increases.

each heuristic. Problems were solved with the network simplex algorithm in CPLEX 9.0 as modeled in (1.1). This provided a global solution for problems with $|\mathbb{V}| \leq 1000$ (larger instances were beyond this technique). Other CPLEX options were considered, but the network simplex method consistently outperformed the other possibilities.

The discrete Lloyd algorithm dominates the other techniques with respect to speed, but as Figure 3 indicates, the solution quality is not as impressive as Hansen's approach, which is routinely within 5% of the global optimum. We wondered if the solution from the discrete Lloyd algorithm could seed the vertex substitution techniques to improve run time. This led to 6 heuristics for each problem and starting point: Maranzana's algorithm, the discrete Lloyd algorithm, Hansen's algorithm, Whitaker's algorithm, and both Hansen's and Whitaker's technique initialized with the solution from the discrete Lloyd algorithm. All implementations were written in MATLAB, and results are reported in terms of the mean and standard deviation of the objective value, number of iterations, and run times over the 30 solves for each problem.

The results for problem instances of size $|\mathbb{V}| = 500$ are shown in Table 1. Tables for all cases are found at `holderfamily.dot5hosting.com/aholder/research/papers/MedianTables.pdf`. The numbers in parentheses indicate the percentage of the global solution found by the network simplex algorithm. For example, a value of (1.10) in the Objective column indicates the heuristic terminated with an objective value that was 110% of the global optimum and a value of (0.72) in the time column means the heuristic required 72% of the time needed to find the global solution.

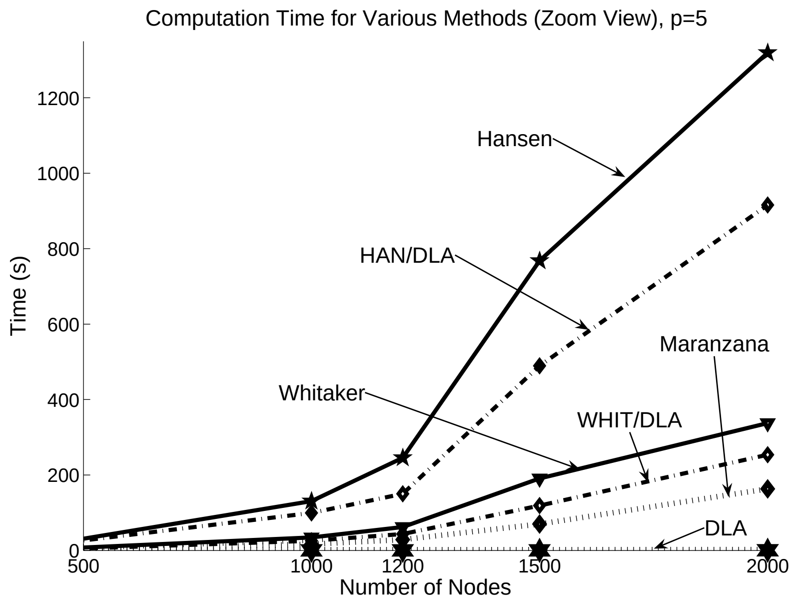

Figure 4: The computation time for the heuristics plotted versus $|\mathbb{V}|$.

Our numerical results mirror the complexity analysis of the previous section and show that the discrete Lloyd algorithm has a computational advantage over the Maranzana algorithm, see Figures 4 and 5. Figure 5 is the same as Figure 4 except that it includes the solution time for the network simplex algorithm for $|\mathbb{V}| \leq 500$, which appears exponential. The heuristics dominate the global approach with respect to speed, although for a few of the smaller networks the heuristics were slower, something we attribute to the MATLAB implementation.

Figure 6 shows an odd trend in the solution quality of the discrete Lloyd and Maranzana algorithms. Allowing $|\mathbb{V}|$ to remain constant, the solution quality degrades as p increases. The ratios of Whitaker and Hansen are nearly constant at 1.02 and 1.3, respectively. This indicates that vertex substitution is less sensitive to a change in p. Each technique took longer to converge as p increased, although the change for the discrete Lloyd method was insignificant.

In general, Hansen's approach obtains excellent solutions but is not as expedient as the other methods. Whitaker's approach is faster but produces solutions of lesser quality. The discrete Lloyd and Maranzana methods are even faster and produce solutions generally better than Whitaker's method. However, these techniques are sensitive to p, and it appears as though solution quality approaches that of Whitaker's approach as p increases. In many cases initializing Whitaker's method with the solution from the Lloyd algorithm improved the solution quality, although the improved solution was still not as good as that from Hansen's technique. Initial-

			Objective		Iterations		Time	
$\|\mathbb{V}\|$	p	Method	μ	σ	μ	σ	μ	σ
		Global	501407.97 (—)	—	114294	—	4282.88 (—)	—
		MAR	549777.60 (1.10)	26591.23	4.13	1.25	2.15 (0.00)	0.12
		DLA	549777.60 (1.10)	26591.23	4.13	1.25	0.03 (0.00)	0.01
500	5	HAN	511191.39 (1.02)	7201.95	9.87	2.11	31.22 (0.01)	6.24
		WHIT	648306.88 (1.29)	50385.48	4.27	2.42	7.61 (0.00)	2.62
		HAN / DLA	511004.83 (1.02)	8521.28	8.00	2.84	26.56 (0.01)	10.64
		WHIT / DLA	545965.52 (1.09)	19918.92	1.33	0.61	5.34 (0.00)	1.29
		Global	274236.58 (—)	—	30483	—	299.22 (—)	—
		MAR	311046.20 (1.13)	16103.83	5.20	1.94	3.09 (0.01)	0.74
		DLA	311046.20 (1.13)	16103.83	5.20	1.94	0.12 (0.00)	0.07
500	10	HAN	278217.88 (1.01)	3492.21	17.87	3.51	216.63 (0.72)	90.27
		WHIT	392236.36 (1.43)	19055.32	7.47	3.41	34.08 (0.11)	20.24
		HAN / DLA	277250.25 (1.01)	3842.16	13.10	4.17	161.88 (0.54)	79.07
		WHIT / DLA	309458.05 (1.13)	14132.92	1.17	0.38	14.61 (0.05)	6.13
		Global	209176.79 (—)	—	142286	—	7465.60 (—)	—
		MAR	241080.60 (1.15)	11371.49	4.57	1.19	2.68 (0.00)	1.01
		DLA	241080.60 (1.15)	11371.49	4.57	1.19	0.11 (0.00)	0.07
500	15	HAN	213132.48 (1.02)	1963.72	23.47	4.06	329.44 (0.04)	171.43
		WHIT	276778.90 (1.32)	13252.56	12.40	3.91	55.78 (0.01)	40.46
		HAN / DLA	213871.82 (1.02)	2478.79	15.73	4.60	234.54 (0.03)	157.51
		WHIT / DLA	238216.37 (1.14)	9649.00	1.63	0.85	19.59 (0.00)	14.52
		Global	167475.09 (—)	—	31609	—	3427.54 (—)	—
		MAR	198087.25 (1.18)	6001.96	4.77	1.25	3.61 (0.00)	0.81
		DLA	198087.25 (1.18)	6001.96	4.77	1.25	0.26 (0.00)	0.11
500	20	HAN	171428.21 (1.02)	1849.10	28.63	4.96	939.15 (0.27)	172.05
		WHIT	219462.79 (1.31)	8785.06	16.80	5.37	184.54 (0.05)	61.14
		HAN / DLA	171983.64 (1.03)	2228.37	20.37	5.01	706.38 (0.21)	186.52
		WHIT / DLA	193251.61 (1.15)	4651.41	2.87	1.38	47.11 (0.01)	19.43
		Global	121038.81 (—)	—	14912	—	795.63 (—)	—
		MAR	151675.27 (1.25)	5472.31	5.17	1.23	3.32 (0.00)	0.46
		DLA	151675.27 (1.25)	5472.31	5.17	1.23	0.37 (0.00)	0.11
500	30	HAN	123840.27 (1.02)	954.77	37.93	3.52	1942.48 (2.44)	249.03
		WHIT	157963.85 (1.31)	4979.40	23.60	6.03	331.29 (0.42)	108.69
		HAN / DLA	124195.91 (1.03)	1284.02	27.70	5.03	1414.40 (1.78)	307.38
		WHIT / DLA	144139.45 (1.19)	3200.81	5.53	2.40	96.13 (0.12)	32.92

Table 1: Data on problem instances with $|\mathbb{V}| = 500$ and varying values of p and solution methods. The number of runs of each heuristic technique was 30.

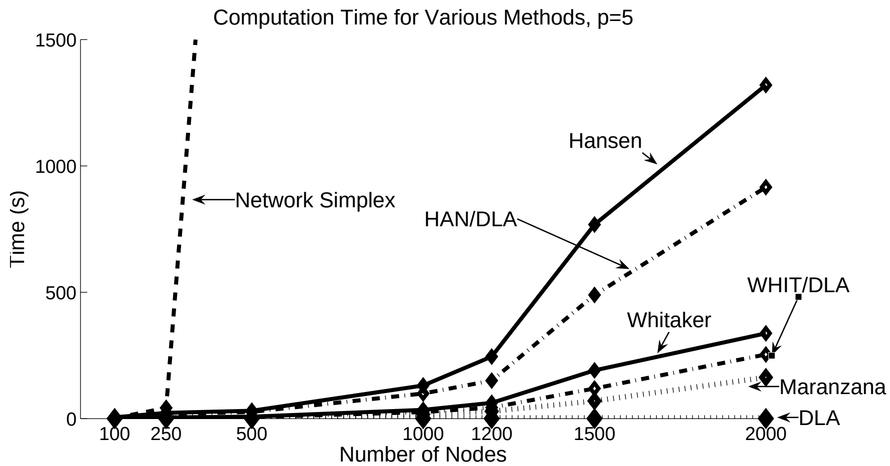

Figure 5: The computation time plotted versus the value of $|\mathbb{V}|$. The solve time for the network simplex algorithm with $|\mathbb{V}| = 1000$ was 675021.47sec $\approx$ 8days

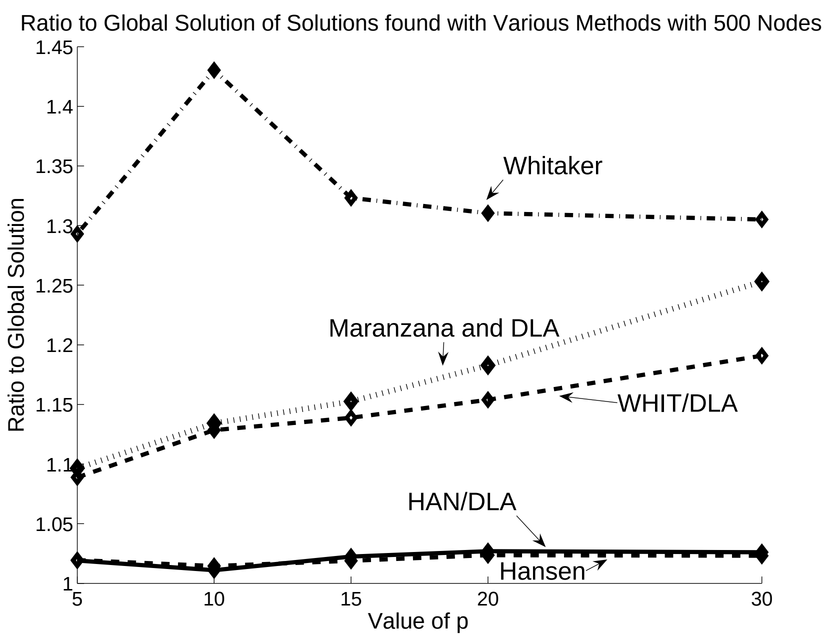

Figure 6: The objective value as a ratio of the global solution versus p with $|\mathbb{V}| = 500$.

izing Hansen's technique with the solution from the discrete Lloyd algorithm did not produce a remarkable change, which is expected since the solutions were generally close to optimal.

In the future we hope to improve the solution quality of the discrete Lloyd algorithm without sacrificing its favorable speed. In particular, we hope to be able to initialize the algorithm so that it converges to a near optimal solution.

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