Entropy Regularized Power $k$-Means Clustering

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Abstract

Despite its well-known shortcomings, $k$-means remains one of the most widely used approaches to data clustering. Current research continues to tackle its flaws while attempting to preserve its simplicity. Recently, the power $k$-means algorithm was proposed to avoid trapping in local minima by annealing through a family of smoother surfaces. However, the approach lacks theoretical justification and fails in high dimensions when many features are irrelevant. This paper addresses these issues by introducing entropy regularization to learn feature relevance while annealing. We prove consistency of the proposed approach and derive a scalable majorization-minimization algorithm that enjoys closed-form updates and convergence guarantees. In particular, our method retains the same computational complexity of $k$-means and power $k$-means, but yields significant improvements over both. Its merits are thoroughly assessed on a suite of real and synthetic data experiments.

1 Introduction

Clustering is a fundamental task in unsupervised learning for partitioning data into groups based on some similarity measure. Perhaps the most popular approach is $k$-means clustering (MacQueen, 1967): given a dataset $\mathcal{X} = \{x_1, \ldots, x_n\} \subset \mathbb{R}^p$, $\mathcal{X}$ is to be partitioned into $k$ mutually exclusive classes so that the variance within each cluster is minimized. The problem can be cast as minimization of the objective

$$P(\Theta) = \sum_{i=1}^{n} \min_{1 \leq j \leq k} \|x_i - \theta_j\|^2,$$

\[ (1) \]
where $\Theta = \{\theta_1, \theta_2, \ldots, \theta_k\}$ denotes the set of cluster centroids, and $\|x_i - \theta_j\|^2$ is the usual squared Euclidean distance metric.

Lloyd’s algorithm (Lloyd, 1982), which iterates between assigning points to their nearest centroid and updating each centroid by averaging over its assigned points, is the most frequently used heuristic to solve the preceding minimization problem. Such heuristics, however, suffer from several well-documented drawbacks. Because the task is NP-hard (Aloise et al., 2009), Lloyd’s algorithm and its variants seek to approximately solve the problem and are prone to stopping at poor local minima, especially as the number of clusters $k$ and dimension $p$ grow. Many new variants have since contributed to a vast literature on the topic, including spectral clustering (Ng et al., 2002), Bayesian (Lock and Dunson, 2013) and non-parametric methods (Kulis and Jordan, 2012), subspace clustering (Vidal, 2011), sparse clustering (Witten and Tibshirani, 2010), and convex clustering (Chi and Lange, 2015); a more comprehensive overview can be found in Jain (2010).

None of these methods have managed to supplant $k$-means clustering, which endures as the most widely used approach among practitioners due to its simplicity. Some work instead focuses on “drop-in” improvements of Lloyd’s algorithm. The most prevalent strategy is clever seeding: $k$-means++ (Arthur and Vassilvitskii, 2007; Ostrovsky et al., 2012) is one such effective wrapper method in theory and practice, and proper initialization methods remain an active area of research (Celebi et al., 2013; Bachem et al., 2016). Geometric arguments have also been employed to overcome sensitivity to initialization. Zhang et al. (1999) proposed to replace the minimum function by the harmonic mean function to yield a smoother objective function landscape but retain a similar algorithm, though the strategy fails in all but very low dimensions. Xu and Lange (2019) generalized this idea by using a sequence of successively smoother objectives via power means instead of the harmonic mean function to obtain better approximating functions in each iteration. The contribution of power $k$-means is algorithmic in nature—it effectively avoids local minima from an optimization perspective, and succeeds for large $p$ when the data points are well-separated. However, it does not address the statistical challenges in high-dimensional settings and performs as poorly as standard $k$-means in such settings. A meaningful similarity measure plays a key role in revealing clusters (De Amorim and Mirkin, 2012; Chakraborty and Das, 2017), but pairwise Euclidean distances become increasingly informative as the number of features grows due to the curse of dimensionality.

On the other hand, there is a rich literature on clustering in high dimensions, but standard approaches such as subspace clustering are not scalable due to the use of an affinity matrix pertaining to norm regularization (Ji et al., 2014; Liu et al., 2012). For spectral clustering, even the creation of such a matrix quickly becomes intractable for modern, large-scale problems (Zhang et al., 2019). Toward learning effective feature representations, Huang et al. (2005) proposed weighted $k$-means clustering ($WK$-means), and sparse
\( k \)-means (Witten and Tibshirani, 2010) has become a benchmark feature selection algorithm, where selection is achieved by imposing \( \ell_1 \) and \( \ell_2 \) constraints on the feature weights. Further related developments can be found in the works of Modha and Spangler (2003); Li and Yu (2006); Huang et al. (2008); De Amorim and Mirkin (2012); Jin and Wang (2016). These approaches typically lead to complex optimization problems in terms of transparency as well as computational efficiency—for instance, sparse \( k \)-means requires solving constrained sub-problems via bisection to find the necessary dual parameters \( \lambda^* \) in evaluating the proximal map of the \( \ell_1 \) term. As they fail to retain the simplicity of Lloyd’s algorithm for \( k \)-means, they lose appeal to practitioners. Moreover, these works on feature weighing and selection do not benefit from recently algorithmic developments as mentioned above.

In this article, we propose a scalable clustering algorithm for high dimensional settings that leverages recent insights for avoiding poor local minima, performs adaptive feature weighing, and preserves the low complexity and transparency of \( k \)-means. Called Entropy Weighted Power \( k \)-means (EWP), we extend the merits of power \( k \)-means to the high-dimensional case by introducing feature weights together with entropy incentive terms. Entropy regularization is not only effective both theoretically and empirically, but leads to an elegant algorithm with closed form solution updates. The idea is to minimize along a continuum of smooth surrogate functions that gradually approach the \( k \)-means objective, while the feature space also gradually adapts so that clustering is driven by informative features. By transferring the task onto a sequence of better-behaved optimization landscapes, the algorithm fares better against the curse of dimensionality and against adverse initialization of the cluster centroids than existing methods. The following summarizes our main contributions:

- We propose a clustering framework that automatically learns a weighted feature representation while simultaneously avoiding local minima through annealing.
- We develop a scalable Majorization-Minimization (MM) algorithm to minimize the proposed objective function.
- We establish descent and convergence properties of our method and prove the strong consistency of the global solution.
- Through an extensive empirical study on real and simulated data, we demonstrate the efficacy of our algorithm, finding that it outperforms comparable classical and state-of-the-art approaches.

The rest of the paper is organized as follows. After reviewing some necessary background, Section 2.1 formulates the Entropy Weighted Power \( k \)-means (EWP) objective and provides high-level intuition. Next,
The principle of MM has become increasingly popular for large-scale optimization in statistical learning (Mairal, 2015; Lange, 2016). Rather than minimizing an objective of interest \( f(\cdot) \) directly, an MM algorithm successively minimizes a sequence of simpler surrogate functions \( g(\theta | \theta_n) \) that majorize the original objective \( f(\theta) \) at the current estimate \( \theta_m \). Majorization requires two conditions: tangency \( g(\theta_m | \theta_m) = f(\theta_m) \) at the current iterate, and domination \( g(\theta | \theta_m) \geq f(\theta) \) for all \( \theta \). The
iterates of the MM algorithm are defined by the rule

$$\theta_{m+1} := \arg\min_{\theta} g(\theta \mid \theta_m)$$  \hspace{1cm} (2)

which immediately implies the descent property

$$f(\theta_{m+1}) \leq g(\theta_{m+1} \mid \theta_m) \leq g(\theta_m \mid \theta_m) = f(\theta_m).$$

That is, a decrease in $g$ results in a decrease in $f$. Note that $g(\theta_{m+1} \mid \theta_m) \leq g(\theta_m \mid \theta_m)$ does not require $\theta_{m+1}$ to minimize $g$ exactly, so that any descent step in $g$ suffices. The MM principle offers a general prescription for transferring a difficult optimization task onto a sequence of simpler problems (Lange et al., 2000), and includes the well-known EM algorithm for maximum likelihood estimation under missing data as a special case (Becker et al., 1997).

**Power k-means** Zhang et al. (1999) attempt to reduce sensitivity to initialization in $k$-means by minimizing the criterion

$$\sum_{i=1}^{n} \left( \frac{1}{k} \sum_{j=1}^{k} \|x_i - \theta_j\|^{-2} \right)^{-1} := f_{-1}(\Theta).$$  \hspace{1cm} (3)

Known as $k$-harmonic means, the method replaces the min appearing in (1) by the harmonic average to yield a smoother optimization landscape, an effective approach in low dimensions. Recently, power $k$-means clustering extends this idea to work in higher dimensions where (3) is no longer a good proxy for (1). Instead of considering only the closest centroid or the harmonic average, the power mean between each point and all $k$ centroids provides a family of successively smoother optimization landscapes. The power mean of a vector $y$ is defined $M_s(y) = \left( \frac{1}{k} \sum_{i=1}^{k} y_i^s \right)^{1/s}$. Within this class, $s > 1$ corresponds to the usual $\ell_1$-norm of $y$, $s = 1$ to the arithmetic mean, and $s = -1$ to the harmonic mean.

Power means enjoy several nice properties that translate to algorithmic merits and are useful for establishing theoretical guarantees. They are monotonic, homogeneous, and differentiable with gradient

$$\frac{\partial}{\partial y_j} M_s(y) = \left( \frac{1}{k} \sum_{i=1}^{k} y_i^s \right)^{\frac{1}{s}-1} \frac{1}{k} y_j^{s-1},$$  \hspace{1cm} (4)

and satisfy the limits

$$\lim_{s \to -\infty} M_s(y) = \min\{y_1, \ldots, y_k\}$$  \hspace{1cm} (5a)

$$\lim_{s \to \infty} M_s(y) = \max\{y_1, \ldots, y_k\}.$$  \hspace{1cm} (5b)

Further, the well-known power mean inequality $M_s(y) \leq M_t(y)$ for any $s \leq t$ holds (Steele, 2004).
The power $k$-means objective function for a given power $s$ is given by the formula

$$f_s(\Theta) = \sum_{i=1}^{n} M_s(\|x_i - \theta_1\|^2, \ldots, \|x_i - \theta_k\|^2).$$  \hfill (6)

The algorithm then seeks to minimize $f_s$ iteratively while sending $s \to -\infty$. Doing so, the objective approaches $f_{-\infty}(\Theta)$ due to (5), coinciding with the original $k$-means objective and retaining its interpretation as minimizing within-cluster variance. The intermediate surfaces provide better optimization landscapes that exhibit fewer poor local optima than (1). Each minimization step is carried out via MM; see Xu and Lange (2019) for details.

2 Entropy Weighted Power $k$-means

A Motivating Example We begin by considering a synthetic dataset with $k = 20$ clusters, $n = 1000$ points, and $p = 100$. Of the 100 features, only 5 are relevant for distinguishing clusters, while the others are sampled from a standard normal distribution (further details are described later in Simulation 2 of Section 4.1). We compare standard $k$-means, WK-means, power $k$-means, and sparse $k$-means with our proposed method; sparse $k$-means is tuned using the gap statistic described in the original paper (Witten and Tibshirani, 2010) as implemented in the R package, sparcl. Figure 1 displays the solutions in a $t$-distributed Stochastic Neighbourhood Embedding (t-SNE) (Maaten and Hinton, 2008) for easy visualization in two dimensions. It is evident that our EWP algorithm, formulated below, yields perfect recovery while the peer algorithms fail to do so. This transparent example serves to illustrate the need for an approach that simultaneously avoids poor local solutions while accommodating high dimensionality.

2.1 Problem Formulation

Let $x_1, \ldots, x_n \in \mathbb{R}^p$ denote the $n$ data points, and $\Theta_{k \times p} = [\theta_1, \ldots, \theta_k]^\top$ denote the matrix whose rows contain the cluster centroids. We introduce a feature relevance vector $w \in \mathbb{R}^p$ where $w_l$ contains the weight of the $l$-th feature, and require these weights to satisfy the constraints

$$\sum_{l=1}^{p} w_l = 1; \quad w_l \geq 0 \text{ for all } l = 1, \ldots, p. \quad \hfill (C)$$

The EWP objective for a given $s$ is now given by

$$f_s(\Theta, w) = \sum_{i=1}^{n} M_s(\|x - \theta_1\|^2, \ldots, \|x - \theta_k\|^2) + \lambda \sum_{l=1}^{p} w_l \log w_l,$$

where the weighted norm $\|y\|^2_w = \sum_{l=1}^{p} w_l y_l^2$ now appears as arguments to the power mean $M_s$. The final term is the negative entropy of $w$ (Jing et al., 2007). This entropy incentive is minimized when $w_l = 1/p$. 6
for all \(l = 1, \ldots, p\); in this case, equation (7) is equal to the power \(k\)-means objective, which in turn equals the \(k\)-means objective when \(s \to -\infty\) (and coincides with KHM for \(s = -1\)). EWP thus generalizes these approaches, while newly allowing features to be adaptively weighed throughout the clustering algorithm. Moreover, we will see in Section 2.2 that entropy incentives are an ideal choice of regularizer in that they lead to closed form updates for \(w\) and \(\theta\) within an iterative algorithm.

**Intuition and the curse of dimensionality** Power \(k\)-means combats the curse of dimensionality by providing smoothed objective functions that remain appropriate as dimension increases. Indeed, in practice the value of \(s\) at convergence of power \(k\)-means becomes lower as the dimension increases, explaining its outperformance over \(k\)-harmonic means (Zhang et al., 1999)\(— f_{-1}\) deteriorates as a reasonable approximation of \(f_{-\infty}\). However even if poor solutions are successfully avoided from the algorithmic perspective, the curse of dimensionality still affects the arguments to the objective. Minimizing within-cluster variance becomes less meaningful as pairwise Euclidean distances become uninformative in high dimensions (Aggarwal et al., 2001). It is therefore desirable to reduce the effective dimension in which distances are computed.

While the entropy incentive term does not zero out variables, it weighs the dimensions according to how useful they are in driving clustering. When the data live in a high-dimensional space yet only a small number of features are relevant towards clustering, the optimal solution to our objective (7) assigns non-negligible weights to only those few relevant features, while benefiting from annealing through the weighted power mean surfaces.

### 2.2 Optimization

To optimize the EWP objective, we develop an MM algorithm (Lange, 2016) for sequentially minimizing (7). As shown by Xu and Lange (2019), \(M_s(y)\) is concave if \(s < 1\); in particular, it lies below its tangent plane. This observation provides the following inequality: denoting \(y_m\) the estimate of a variable \(y\) at iteration \(m\),

\[
M_s(y) \leq M_s(y_m) + \nabla_y M_s(y_m)^	op (y - y_m) \tag{8}
\]

Substituting \(\|x_i - \theta_j\|_{w_m}^2\) for \(y_j\) and \(\|x_i - \theta_{mj}\|_{w_m}^2\) for \(y_{m,j}\) in equation (8) and summing over all \(i\), we obtain

\[
f_s(\Theta, w) \leq f_s(\Theta_m, w_m) - \sum_{i=1}^n \sum_{j=1}^k \phi^{(m)}_{ij} \|x_i - \theta_{mj}\|_{w_m}^2 \\
- \lambda \sum_{l=1}^p (w_{m,l} \log w_{m,l} - w_l \log w_l) + \sum_{i=1}^n \sum_{j=1}^k \phi^{(m)}_{ij} \|x_i - \theta_j\|_{w}^2.
\]

7
Here the derivative expressions (4) provide the values of the constants
\[
\phi_{ij}^{(m)} = \frac{\frac{1}{k} x_i - \theta_{m,j}}{\sum_{j=1}^{k} ||x_i - \theta_{m,j}||^2_{w_m} (1 - 2s)}.
\]
The right-hand side of the inequality above serves as a \emph{surrogate function} majorizing \(f_s(\Theta, w)\) at the current estimate \(\Theta_m\). Minimizing this surrogate amounts to minimizing the expression
\[
\sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij}^{(m)} ||x_i - \theta_j||^2_{w_m} + \lambda \sum_{l=1}^{p} w_l \log w_l \tag{9}
\]
subject to the constraints (C). This problem admits closed form solutions: minimization over \(\Theta\) is straightforward, and the optimal solutions are given by
\[
\theta^*_j = \sum_{i=1}^{n} \phi_{ij} x_i \sum_{i=1}^{n} \phi_{ij}.
\]
To minimize equation (9) in \(w\), we consider the Lagrangian
\[
\mathcal{L} = \sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij} ||x_i - \theta_j||^2_{w} + \lambda \sum_{l=1}^{p} w_l \log w_l - \alpha (\sum_{l=1}^{p} w_l - 1).
\]
The optimality condition \(\frac{\partial \mathcal{L}}{\partial w_l} = 0\) implies \(\sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij} (x_{il} - \theta_{jl})^2 + \lambda (1 + \log w_l) - \alpha = 0\). This further implies that
\[
w^*_l \propto \exp \left\{ - \sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij} (x_{il} - \theta_{jl})^2 \right\}.
\]
Now enforcing the constraint \(\sum_{l=1}^{p} w_l = 1\), we get
\[
w^*_l = \frac{\exp \left\{ - \sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij} (x_{il} - \theta_{jl})^2 \right\}}{\sum_{l=1}^{p} \exp \left\{ - \sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij} (x_{il} - \theta_{jl})^2 \right\}}
\]
Thus, the MM steps take a simple form and amount to two alternating updates:
\[
\theta_{m+1,j} = \frac{\sum_{i=1}^{n} \phi_{ij}^{(m)} x_i}{\sum_{i=1}^{n} \phi_{ij}^{(m)}} \tag{10}
\]
\[
w_{m+1,l} = \frac{\exp \left\{ - \sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij}^{(m)} (x_{il} - \theta_{jl})^2 \right\}}{\sum_{l=1}^{p} \exp \left\{ - \sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij}^{(m)} (x_{il} - \theta_{jl})^2 \right\}} \tag{11}
\]
The MM updates are similar to those in Lloyd’s algorithm (Lloyd, 1982) in the sense that each step alternates between updating \(\phi_{ij}\)’s and updating \(\Theta\) and \(w\). These updates are summarised in Algorithm 1; though there are three steps rather than two, the overall per-iteration complexity of this algorithm is the same as that
of \(k\)-means (and power \(k\)-means) at \(O(nkp)\) (Lloyd, 1982). We require the tuning parameter \(\lambda > 0\) to be specified, typically chosen via cross-validation detailed in Section 4.1. It should be noted that the initial value \(s_0\) and the constant \(\eta\) do not require careful tuning: we fix them at \(s_0 = -1\) and \(\eta = 1.05\) across all real and simulated settings considered in this paper.

\textbf{Algorithm 1:} Entropy Weighted Power \(k\)-means Algorithm (EWP)

\begin{verbatim}
Data: \(X \in \mathbb{R}^{n \times p}\), \(\lambda > 0\), \(\eta > 1\)
Result: \(\Theta\)
initialize \(s_0 < 0\) and \(\Theta_0\)
repeat:
\[ \phi_{ij}^{(m)} \leftarrow \frac{1}{k} ||x_i - \theta_{m,j}||^2 (s_m - 1) \left( \frac{1}{k} \sum_{j=1}^{k} ||x_i - \theta_{m,j}||^2 s_m \right)^{\frac{1}{s_m} - 1} \]
\[ \theta_{m+1,j} \leftarrow \frac{\sum_{i=1}^{n} \phi_{ij}^{(m)} x_i}{\sum_{i=1}^{n} \phi_{ij}^{(m)}} \]
\[ w_{m+1,l} \leftarrow \exp \left\{ -\frac{\sum_{i=1}^{n} \sum_{j=1}^{k} \phi_{ij}^{(m)} (x_{il} - \theta_{jl})^2}{\lambda} \right\} \]
\[ s_{m+1} \leftarrow \eta s_m \]
until convergence
\end{verbatim}

3 Theoretical Properties

We note that all iterates \(\theta_m\) in Algorithm 1 are defined within the convex hull of the data, all weight updates lie within \([0, 1]\), and the procedure enjoys convergence guarantees as an MM algorithm (Lange, 2016). Before we state and prove the main result of this section on strong consistency, we present results characterizing the sequence of minimizers. Theorems 1 and 2 show that the minimizers of surfaces \(f_s\) always lie in the convex hull of the data \(C^k\), and converge uniformly to the minimizer of \(f_{-\infty}\).

\textbf{Theorem 1.} Let \(s \leq 1\) also let \((\Theta_{n,s}, w_{n,s})\) be minimizer of \(f_s(\Theta, w)\). Then we have \(\Theta_{n,s} \in C^k\).

\textbf{Proof.} Let \(P_C^w(\theta)\) denote the projection of \(\theta\) onto \(C\) w.r.t. the \(||\cdot||_w\) norm. Now for any \(v \in C\), using the
obtise angle condition, we obtain, 

\[ \langle \theta - P_C^w(\theta), v - P_C^w(\theta) \rangle_w \leq 0. \]

Since \( x_i \in C \), we obtain,

\[
\|x_i - \theta_j\|_w^2 = \|x_i - P_C^w(\theta_j)\|_w^2 + \|P_C^w(\theta_j) - \theta_j\|_w^2 \\
- 2\langle \theta - P_C^w(\theta_j), x_i - P_C^w(\theta_j) \rangle_w \\
\geq \|x_i - P_C^w(\theta_j)\|_w^2 + \|P_C^w(\theta_j) - \theta_j\|_w^2.
\]

Now since, \( M_s(\cdot) \) is an increasing function in each of its argument, if we replace \( \theta_j \) by \( P_C^w(\theta_j) \) in \( M_s(\|x_i - \theta_1\|_w, \ldots, \|x_i - \theta_k\|_w^2) \), the objective function value doesn’t go up. Thus we can effectively restrict our attention to \( C^k \). Now since the function \( f_s(\cdot, \cdot) \) is continuous on the compact set \( C^k \times [0,1]^p \), it attains its minimum on \( C^k \times [0,1]^p \). Thus, \( \Theta^* \in C^k \).

**Theorem 2.** For any decreasing sequence \( \{s_m\}_{m=1}^\infty \) such that \( s_1 \leq 1 \) and \( s_m \to -\infty \), \( f_{s_m}(\Theta, w) \) converges uniformly to \( f_{-\infty}(\Theta, w) \) on \( C^k \times [0,1]^p \).

**Proof.** For any \( (\Theta, w) \in C^k \times [0,1]^p \), \( f_{s_m}(\Theta, w) \) converges monotonically to \( f_{-\infty}(\Theta, w) \) (this is due to the power mean inequality). Since \( C^k \times [0,1]^p \) is compact, the result follows immediately upon applying Dini’s theorem from real analysis.

Strong consistency is a fundamental requirement of any “good” estimator in the statistical sense: as the number of data points grows, one should be able to recover true parameters with arbitrary precision (Terada, 2014, 2015; Chakraborty and Das, 2019). The proof of our main result builds upon the core argument for k-means consistency by Pollard (1981), and extends the argument through novel arguments involving uniform convergence of the family of annealing functions.

Let \( x_1, \ldots, x_n \in \mathbb{R}^p \) be independently and identically distributed from distribution \( P \) with support on a compact set \( C \subset \mathbb{R}^p \). For notational convenience, we write \( M_s(x, \Theta, w) \) for \( M_s(\|x - \theta_1\|_w, \ldots, \|x - \theta_k\|_w) \).

We consider the following minimization problem

\[
\min_{\theta, w} \left\{ \frac{1}{n} \sum_{i=1}^n M_s(x_i, \Theta, w) + \lambda \sum_{l=1}^p w_l \log w_l \right\},
\]

which is nothing but a scaled version of equation (7). Intuitively, as \( n \to \infty \), \( \frac{1}{n} \sum_{i=1}^n M_s(x_i, \Theta, w) \) is very close to \( \int M_s(x, \Theta, w)dP \) almost surely by appealing to the Strong Law of Large Numbers (SLLN). Together with (5), as \( n \to \infty \) and \( s \to -\infty \) we expect

\[
\frac{1}{n} \sum_{i=1}^n M_s(x_i, \Theta, w) + \lambda \sum_{l=1}^p w_l \log w_l 
\]

(12)

to be in close proximity of

\[
\int \min_{\theta \in \Theta} \|x - \theta\|_w dP + \lambda \sum_{l=1}^p w_l \log w_l,
\]

(13)
so that minimizers of the (12) should be very close to the minimizers of (13) under certain regularity conditions.

To formalize this intuition, let $\Theta^*$, $w^*$ be minimizers of

$$
\Phi(\Theta, w) = \int \min_{1 \leq j \leq k} \|x - \theta_j\|_w^2 dP + \lambda \sum_{l=1}^{p} w_l \log w_l,
$$

and define $\Theta_{n,s}$, $w_{n,s}$ as the minimizers of

$$
\int \mathcal{M}_s(x, \Theta, w) dP_n + \lambda \sum_{l=1}^{p} w_l \log w_l,
$$

where $P_n$ is the empirical measure. We will show that $\Theta_{n,s} \xrightarrow{a.s.} \Theta^*$ and $w_{n,s} \xrightarrow{a.s.} w^*$ as $n \to \infty$ and $s \to -\infty$ under the following identifiability assumption:

A1 For any neighbourhood $N$ of $(\Theta^*, w^*)$, there exists $\eta > 0$ such that if $(\Theta, w) \notin N$ implies that $\Phi(\Theta, w) > \Phi(\Theta^*, w^*) + \eta$.

Theorem 3 establishes a uniform SLLN, which plays a key role in the proof of the main result (Theorem 4).

**Theorem 3. (SLLN)** Fix $s \leq 1$. Let $\mathcal{G}$ denote the family of functions $g_{\Theta, w}(x) = \mathcal{M}_s(x, \Theta, w)$. Then $\sup_{g \in \mathcal{G}} |\int g dP_n - \int g dP| \to 0$ a.s. $[P].$

**Proof.** Fix $\epsilon > 0$. It is enough to find a finite family of functions $\mathcal{G}_\epsilon$ such that for all $g \in \mathcal{G}$, there exists $\hat{g}, \check{g} \in \mathcal{G}_\epsilon$ such that $g \leq \hat{g} \leq \check{g}$ and $\int (\hat{g} - \check{g}) dP < \epsilon$.

Let us define $\phi(\cdot) : \mathbb{R} \to \mathbb{R}$ such that $\phi(x) = \max\{0, x\}$. Since $C$ is compact, for every $\delta_1 > 0$, we can always construct a finite set $C_{\delta_1} \subset C$ such that if $\theta \in C$, there exist $\theta' \in C_{\delta_1}$ such that $\|\theta - \theta'\| < \delta_1$. Similarly, resorting to the compactness of $[0, 1]^p$, for every $\delta_2 > 0$, we can always construct a finite set $W_{\delta_2} \subset [0, 1]^p$ such that if $w \in [0, 1]^p$, there exist $w' \in W_{\delta_2}$ such that $\|w - w'\| < \delta_2$. Consider the function $h(x, \Theta, w) = M_s(\|x - \theta_1\|_w^2, \ldots, \|x - \theta_k\|_w^2)$ on $C \times C^k \times [0, 1]^p$. $h$, being continuous on the compact set $C \times C^k \times [0, 1]^p$, is also uniformly continuous. Thus for all $x \in C$, if $\|w - w'\| < \delta_2$ and $\|\theta_j - \theta'_j\| < \delta_1$ for all $j = 1, \ldots, k$ implies that

$$
M_s(\|x - \theta_1\|_w^2, \ldots, \|x - \theta_k\|_w^2) - M_s(\|x - \theta'_1\|_w^2, \ldots, \|x - \theta'_k\|_w^2) < \epsilon/2 \quad (14)
$$

We take

$$
\mathcal{G}_\epsilon = \{ \phi(M_s(\|x - \theta'_1\|_w^2, \ldots, \|x - \theta'_k\|_w^2) \pm \epsilon/2) : \theta'_1, \ldots, \theta'_k \in C_{\delta_1} \text{ and } w' \in W_{\delta_2} \}.
$$
Now if we take

$$\tilde{g}_{\theta, w} = \phi(M_{s}(\|x - \theta_{1}'\|_{w}, \ldots, \|x - \theta_{k}'\|_{w}) + \epsilon/2)$$

and

$$\hat{g}_{\theta, w} = \phi(M_{s}(\|x - \theta_{1}'\|_{w}, \ldots, \|x - \theta_{k}'\|_{w}) - \epsilon/2),$$

where $\theta_{j}' \in C_{\delta_{1}}$ and $w \in W_{\delta_{2}}$ for $j = 1, \ldots, k$ such that $\|\theta_{j} - \theta_{j}'\| < \delta_{1}$ and $\|w - w'\| < \delta_{2}$. From equation (14), we get, $\hat{g} \leq g \leq \tilde{g}$. Now we need to show $\int (\tilde{g} - \hat{g})dP < \epsilon$. This step is straightforward.

$$\int (\tilde{g} - \hat{g})dP$$

$$= \left[ \phi(M_{s}(\|x - \theta_{1}'\|_{w}, \ldots, \|x - \theta_{k}'\|_{w}) + \epsilon/2) - \phi(M_{s}(\|x - \theta_{1}'\|_{w}, \ldots, \|x - \theta_{k}'\|_{w}) - \epsilon/2) \right] dP$$

$$\leq \epsilon \int dP = \epsilon.$$

Hence the result. \qed

We are now ready to establish the main consistency result, stated and proven below.

**Theorem 4.** Under the condition A1, $\Theta_{n,s} \xrightarrow{a.s.} \Theta^{*}$ and $w_{n,s} \xrightarrow{a.s.} w^{*}$ as $n \to \infty$ and $s \to -\infty$.

**Proof.** It is enough to show that given any neighbourhood $N$ of $(\Theta^{*}, w^{*})$, there exists $M_{1} < 0$ and $M_{2} > 0$ such that if $s < M_{1}$ and $n > M_{2}$ such that $(\Theta, w) \in N$ almost surely. By assumption A1, it is enough to show that for all $\eta > 0$, there exists $M_{1} < 0$ and $M_{2} > 0$ such that if $s < M_{1}$ and $n > M_{2}$ such that $\Phi(\Theta, w) \leq \Phi(\Theta^{*}, w^{*}) + \eta$ almost surely. For notational convenience, we write $M_{s}(\|x - \theta_{1}\|_{w}, \ldots, \|x - \theta_{k}\|_{w})$ and $\alpha(w) = \lambda \sum_{i=1}^{p} w_{i} \log w_{i}$. Now since $(\Theta_{n,s}, w_{n,s})$ is the minimizer for $\int M_{s}(x, \Theta, w)dP_{n} + \lambda \sum_{i=1}^{p} w_{i} \log w_{i}$, we get,

$$\int M_{s}(x, \Theta_{n,s}, w_{n,s})dP_{n} + \lambda \alpha(w_{n,s})$$

$$\leq \int M_{s}(x, \Theta^{*}, w^{*})dP_{n} + \lambda \alpha(w^{*}). \quad (15)$$

Now observe that $\Phi(\Theta_{n,s}, w_{n,s}) - \Phi(\Theta^{*}, w^{*}) = \xi_{1} + \xi_{2} + \xi_{3}$, where,

$$\xi_{1} = \Phi(\Theta_{n,s}, w_{n,s}) - \int M_{s}(x, \Theta_{n,s}, w_{n,s})dP - \lambda \alpha(w_{n,s}),$$

$$\xi_{2} = \int M_{s}(x, \Theta_{n,s}, w_{n,s})dP - \int M_{s}(x, \Theta_{n,s}, w_{n,s})dP_{n},$$

$$\xi_{3} = \int M_{s}(x, \Theta_{n,s}, w_{n,s})dP_{n} + \lambda \alpha(w_{n,s}) - \Phi(\Theta^{*}, w^{*}).$$

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We first choose \( M_1 < 0 \) such that if \( s < M_1 \) then
\[
\left| \min_{1 \leq j \leq k} \| x - \theta_j \|_w - M_s(x, \Theta, w) \right| < \eta/6
\] (16)
for all \( x \in C, \Theta \in C^k \) and \( w \in [0,1]^p \). Thus for \( s < M_1 \), \( \min_{1 \leq j \leq k} \| x - \theta_j \|_w \leq M_s(x, \Theta, w) + \eta/6 \) which in turn implies that \( \int \min_{1 \leq j \leq k} \| x - \theta_j \|_w dP_n \leq \int M_s(x, \Theta, w) dP_n + \eta/3 \). Substituting \( \Theta_{n,s} \) for \( \Theta \) and \( w_{n,s} \) for \( w \) in the above expression and adding \( \lambda \alpha(w_{n,s}) \) to both sides, we get \( \xi_1 < \eta/6 \). We also observe that the quantity \( \xi_2 \) can also be made smaller that \( \eta/3 \) by appealing to the uniform SLLN (Theorem 3). Now to bound \( \xi_3 \), we observe that
\[
\xi_3 \leq \int M_s(x, \Theta^*, w^*) dP_n + \lambda \alpha(w^*) - \Phi(\Theta^*, w^*)
\]
\[
= \int M_s(x, \Theta^*, w^*) dP_n - \int_{\theta \in \Theta^*} \| x - \theta \|_{w^*} dP
\]
This inequality is obtained by appealing to equation (15). Again appealing to the uniform SLLN, we get that for large enough \( n \),
\[
\xi_3 \leq \int M_s(x, \Theta^*, w^*) dP - \int_{\theta \in \Theta^*} \| x - \theta \|_{w^*} dP + \eta/6
\]
\[
\leq \int [\min_{\theta \in \Theta^*} \| x - \theta \|_{w^*} + \eta/6] dP - \int_{\theta \in \Theta^*} \| x - \theta \|_{w^*} dP
\]
\[
+ \eta/6 = \eta/3.
\]
The second inequality follows from equation (16). Thus we get, \( \Phi(\Theta_{n,s}, w_{n,s}) - \Phi(\Theta^*, w^*) = \xi_1 + \xi_2 + \xi_3 \leq \eta/6 + \eta/3 + \eta/3 < \eta \) almost surely. The result now follows.

4 Empirical Performance

We examine the performance of EWP on a variety of simulated and real datasets compared to classical and state-of-the-art peer algorithms. All the datasets and the codes pertaining to this paper are publicly available at [https://github.com/DebolinaPaul/EWP](https://github.com/DebolinaPaul/EWP). For evaluation purposes, we use the Normalized Mutual Information (NMI) ([Vinh et al., 2010](https://doi.org/10.1007/s10897-010-0159-2)) between the ground-truth partition and the partition obtained by each algorithm. A value of 1 indicates perfect clustering and a value of 0 indicates arbitrary labels. As our algorithm is meant to perform as a drop-in replacement to \( k \)-means, we focus comparisons to Lloyd’s classic algorithm ([Lloyd, 1982](https://doi.org/10.1007/BF02842523)), WK-\( k \)-means ([Huang et al., 2005](https://doi.org/10.1007/11549589_9)), Power \( k \)-means ([Xu and Lange, 2019](https://doi.org/10.1007/978-3-030-12203-0_10)), and sparse \( k \)-means ([Witten and Tibshirani, 2010](https://doi.org/10.1007/978-3-642-11546-5_11)). It should be noted that sparse \( k \)-means already entails higher computational complexity, and we do not exhaustively consider alternate methods which require orders of magnitude of higher complexity. In all cases, each algorithm is initiated with the same set of randomly chosen centroids.
4.1 Synthetic Experiments

We now consider a suite of simulation studies to validate the proposed EWP algorithm.

Figure 2: Solutions obtained by the peer algorithms for an example dataset with \( k = 100 \) and \( d = 20 \) in Simulation 1 (4.1). The obtained cluster centroids appear as black diamonds in the figure.

**Simulation 1** The first experiment assesses performance as the dimension and number of uninformative features grows. We generate \( n = 1000 \) observations with \( k = 100 \) clusters. Each observation has \( p = d + 2 \) many features as \( d \) varies between 5 and 100. The first two features reveal cluster structure, while the remaining \( d \) variables are uninformative, generated independently from a \( \text{Unif}(0,2) \) distribution. True centroids are spaced uniformly on a grid with \( \theta_m = \frac{m-1}{10} \), and \( x_{ij} \sim \frac{1}{10} \sum_{m=1}^{10} \mathcal{N}(\theta_m, 0.15) \). Despite the simple data generating setup, clustering is difficult due to the low signal to noise ratio in this setting.

We report the average NMI values between the ground-truth partition and the partition obtained by
Table 1: NMI values for Simulation 1, showing the effect of the number of unimportant features.

|               | $d = 5$      | $d = 10$      | $d = 20$      | $d = 50$      | $d = 100$     |
|---------------|--------------|--------------|--------------|--------------|--------------|
| $k$-means     | 0.3913 (0.002) | 0.3701 (0.002) | 0.3674 (0.003) | 0.3629 (0.002) | 0.3517 (0.003) |
| WK-$k$-means  | 0.5144 (0.002) | 0.50446 (0.003) | 0.5050 (0.003) | 0.5026 (0.005) | 0.5029 (0.003) |
| Power $k$-means | 0.3924 (0.001) | 0.3873 (0.002) | 0.3722 (0.001) | 0.3967 (0.003) | 0.3871 (0.004) |
| Sparse $k$-means | 0.3679 (0.002) | 0.3677 (0.002) | 0.3668 (0.001) | 0.3675 (0.002) | 0.3637 (0.002) |
| EWP-$k$-means | **0.9641** (0.001) | **0.9217** (0.001) | **0.9139** (0.001) | **0.9465** (0.001) | **0.9082** (0.003) |

each of the algorithms over 20 trials in Table 1, with the standard deviations appearing in parentheses. The best performing algorithm in each column appears in bold, and the best solutions for $d = 20$ are plotted in Figure 2. The benefits using EWP are visually stark, and Table 1 verifies in detail that EWP outperforms the classical $k$-means algorithm as well as the state-of-the-art sparse-$k$-means and the power $k$-means algorithms. The inability of $k$-means and Power $k$-means to properly learn the feature weights results in poor performance of these algorithms. On the other hand, although WK-$k$-means and sparse $k$-means can select features successfully, they fail from the optimization perspective when $k$ is large enough so that there are many local minima to trap the algorithm.

**Simulation 2**  We next examine the effect of $k$ on the performance, taking $n = 100 \cdot k$ and $p = 100$ while $k$ varies from 20 to 500. The matrix $\Theta_{k \times p}$, whose rows contain the cluster centroids, is generated as follows.

1. Select 5 relevant features $l_1, \ldots, l_5$ at random.

2. Simulate $\theta_{j,l,m} \sim Unif(0, 1)$ for all $j = 1, \ldots, k$ and $m = 1, \ldots, 5$.

3. Set $\theta_{j,l} = 0$ for all $l \notin \{l_1, \ldots, l_5\}$ and all $j$.

After obtaining $\Theta$, $x_{il}$ is simulated as follows.

$x_{il} \sim \mathcal{N}(0, 1)$ if $l \notin \{l_1, \ldots, l_5\}$

$x_{il} \sim \frac{1}{k} \sum_{j=1}^{k} \mathcal{N}(\theta_{j,l}, 0.015)$ if $l \in \{l_1, \ldots, l_5\}$.

We run each of the algorithms 20 times and report the average NMI values between the ground-truth partition and the partition obtained by each of the algorithms in Table 2; with standard errors appearing in parentheses. Table 2 shows that $k$-means, WK-$k$-means, power $k$-means, and sparse $k$-means lead to almost the same result, while EWP outperforms all the peer algorithms for each $k$ as it narrows down the large number of features and avoids local minima from large $k$ simultaneously.
Table 2: NMI values for Simulation 2, showing the effect of increasing number of clusters.

|             | k = 20        | k = 100       | k = 200       | k = 500       |
|-------------|---------------|---------------|---------------|---------------|
| k-means     | 0.0674(0.001) | 0.2502(0.021) | 0.3399 (0.031) | 0.3559 (0.014) |
| WK-means    | 0.0587(0.001) | 0.2247(0.002) | 0.3584(0.018) | 0.3678(0.009) |
| Power k-means | 0.0681(0.001) | 0.2785(0.001) | 0.3578 (0.002) | 0.3867(0.001) |
| Sparse k-means | 0.0679(0.001) | 0.2490(0.058) | 0.6705(0.007) | 0.3537 (0.002) |
| EWP-k-means | **0.9887(0.001)** | **0.9844 (0.002)** | **0.9756(0.001)** | **0.9908 (0.001)** |

Figure 3: Boxplots show that EWP consistently identifies true features while sparse k-means fails to do so.

**Feature Selection**  We now examine the feature weighting properties of the EWP algorithm more closely. We take n = 1000, p = 20 and follow the same data generation procedure described in Simulation 2. For simplicity, in the first step of the simulation study, we select \( l_i = i \) for \( i = 1, \ldots, 5 \). We record the feature weights obtained by EWP, sparse k-means and WK-means over 100 replicate datasets. The box-plot for these 100 optimal feature weights are shown in Figure 3 for all the three algorithms. The proposed method successfully assigns almost all weight to relevant features 1 through 5, even though it does not make use of a sparsity-inducing penalty. Meanwhile, feature weights assigned by sparse k-means do not follow any clear pattern related to informative features, even though the ground truth is sparse in relevant features. The analogous plot for WK-means shows even worse performance than sparse k-means. The study clearly illustrates the necessity of feature weighing together with annealing for successful k-means clustering in high dimensional settings.
4.2 Case Study and Real Data

We now assess performance on real data, beginning with a case study on Glioma. The GLIOMA dataset consists of 50 datapoints and is divided into 4 classes consisting of cancer glioblastomas (CG), noncancer glioblastomas (NG), cancer oligodendrogliomas (CO) and non-cancer oligodendrogliomas (NO). Each observation consists of 4434 features. The data were collected in the study by Nutt et al. (2003), and are also available by Li et al. (2018). In our experimental studies, we compare the EWP algorithm to the four peer algorithms considered in Section 4.1. In order to visualize clustering solutions, we embed the data into the plane via t-SNE (Maaten and Hinton, 2008). The best partitioning obtained from each algorithm is shown in Figure 4, which makes it visually clear that clustering under EWP more closely resembles the ground truth compared to competitors. This is detailed by average NMI values as well as standard deviations in
parentheses listed in Table 3.

Table 3: Mean NMI and standard deviation, GLIOMA

|        | k-means | WK-means | Power  | Sparse  | EWP     |
|--------|---------|----------|--------|---------|---------|
|        | 0.490 (0.040) | 0.427 (0.034) | 0.499 (0.020) | 0.108 (0.001) | 0.594 (0.001) |

Further real-data experiments To further validate our method in various real data scenarios, we perform a series of experiments on 10 benchmark datasets collected from the UCI machine learning repository (Dua and Graff, 2017), Keel Repository (Alcalá-Fdez et al., 2011) and ASU repository (Li et al., 2018). A brief description of these datasets can be found in Table 4.

Average performances over 20 independent trials are reported in Table 5; the EWP algorithm outperforms by a large margin across all instances when compared to the other peer algorithms. To determine the statistical significance of the results, we employ Wilcoxon’s signed-rank test (Wasserman, 2006) at the 5% level of significance. In Table 5, an entry marked with + (≃) differs from the corresponding result of EWP with statistical significance. Finally, we emphasize that our results comprise a conservative comparison in that parameters $s_0 = -1$ and $\eta = 1.05$ are fixed across all settings. While this demonstrates that careful tuning of these parameters is not necessary for successful clustering, performance can be further improved by doing so (Xu and Lange, 2019),

5 Discussion

Despite decades of advancement on $k$-means clustering, Lloyd’s algorithm remains the most popular choice in spite of its well-known drawbacks. Extensions and variants that address these flaws fail to preserve its simplicity, scalability, and ease of use. Many of these methods still fall short at poor local optima or fail when data are high-dimensional with low signal-to-noise ratio, and few come with rigorous statistical guarantees such as consistency.

The contributions in this paper seek to fill this methodological gap, with a novel formulation that draws from good intuition in classic and recent developments. With emphasis on simplicity as a chief priority, we derive a method that can be seen as a drop-in replacement to Lloyd’s classic $k$-means algorithm, reaping large improvements in practice even when there are a large number of clusters or features in the data. By designing the algorithm from the perspective of MM, our method is robust as a descent algorithm and achieves an ideal $O(n kp)$ complexity. In contrast to popular approaches such as sparse $k$-means and power
Table 4: Source and Description of the Datasets

| Datasets         | Source        | k  | n   | p  |
|------------------|---------------|----|-----|----|
| Iris             | Keel Repository | 3  | 150 | 4  |
| Automobile       | Keel Repository | 6  | 150 | 25 |
| Mammographic     | Keel Repository | 2  | 830 | 5  |
| Newthyroid       | Keel Repository | 3  | 215 | 5  |
| Wine             | Keel Repository | 3  | 178 | 13 |
| WDBC             | Keel Repository | 2  | 569 | 30 |
| Movement Libras  | Keel Repository | 15 | 360 | 90 |
| Wall Robot 4     | UCI Repository | 4  | 5456| 4  |
| WarpAR10P        | ASU Repository | 10 | 130 | 2400|
| WarpPIE10P       | ASU Repository | 10 | 210 | 2420|

Table 5: NMI values on Benchmark Real Data

| Datasets         | k-means      | Power k-means | WK-means    | Sparse k-means | EWP-k-means  |
|------------------|--------------|---------------|-------------|----------------|--------------|
| Newthyroid       | 0.403±(0.002)| 0.262±(0.002)| 0.407±(0.004)| 0.102±(0.002) | 0.5321±(0.003)|
| Automobile       | 0.165±(0.009)| 0.203±(0.010)| 0.168±(0.005)| 0.168±(0.007) | 0.311±(0.003)|
| WarpAR10P        | 0.170±(0.042)| 0.233±(0.031)| 0.201±(0.019)| 0.185±(0.008) | 0.350±(0.047)|
| WarpPIE10P       | 0.240±(0.031)| 0.240±(0.028)| 0.180±(0.022)| 0.179±(0.002) | 0.2761±(0.041)|
| Iris             | 0.758±(0.003)| 0.788±(0.005)| 0.741±(0.005)| 0.813±(0.002) | 0.849±(0.005)|
| Wine             | 0.428±(0.001)| 0.642±(0.005)| 0.416±(0.002)| 0.428±(0.001) | 0.747±(0.003)|
| Mammographic     | 0.107±(0.001)| 0.019±(0.003)| 0.115±(0.001)| 0.110±(0.002) | 0.405±(0.002)|
| WDBC             | 0.463±(0.002)| 0.005±(0.005)| 0.464±(0.002)| 0.467±(0.003) | 0.656±(0.001)|
| LIBRAS           | 0.553±(0.017)| 0.339±(0.020)| 0.461±(0.021)| 0.254±(0.014) | 0.575±(0.009)|
| Wall Robot 4     | 0.167±(0.027)| 0.183±(0.013)| 0.171±(0.030)| 0.186±(0.012) | 0.234±(0.003)|
k-means, the proposed approach is provably consistent.

Extending the intuition to robust measures and other divergences in place of the Euclidean distance are warranted. Further, research toward finite-sample prediction error bounds or convergence rates relating to the annealing schedule will also be fruitful avenues for future work.

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