Compressed *K*-Means for Large-Scale Clustering

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Abstract

Large-scale clustering has been widely used in many applications, and has received much attention. Most existing clustering methods suffer from both expensive computation and memory costs when applied to large-scale datasets. In this paper, we propose a novel clustering method, dubbed compressed k-means (CKM), for fast large-scale clustering. Specifically, high-dimensional data are compressed into short binary codes, which are well suited for fast clustering. CKM enjoys two key benefits: 1) storage can be significantly reduced by representing data points as binary codes; 2) distance computation is very efficient using Hamming metric between binary codes. We propose to jointly learn binary codes and clusters within one framework. Extensive experimental results on four large-scale datasets, including two million-scale datasets demonstrate that CKM outperforms the state-of-the-art large-scale clustering methods in terms of both computation and memory cost, while achieving comparable clustering accuracy.

Introduction

Clustering is a fundamental technique in machine learning and pattern recognition. The aim of clustering is to partition a data set into different groups with similar data points being assigned into one group. Until now many clustering algorithms (Hartigan and Wong 1979; Ng et al. 2001; Li et al. 2009; Wang et al. 2011b; Ding et al. 2015) have been proposed, including the widely used k-means clustering (Hartigan and Wong 1979; Arthur and Vassilvitskii 2007; Ding et al. 2015) and spectral clustering (Shi and Malik 2000; Ng et al. 2001).

There has been a dramatic growth in the volume of data with the advent of Internet in the recent decades. For instance, Flickr has more than 5 billion images available, YouTube receives more than 100 hours of videos uploaded per minute. Conventional clustering methods such as spectral clustering cannot be directly applied to large-scale datasets due to their high computation cost. Recently, increased attention has been paid to large-scale clustering (Chen and Cai 2011; Chen et al. 2011; Li et al. 2015; Gong et al. 2015; Zhang and Lu 2016), which aims to develop clustering methods with high scalability. For example, several variants, e.g., Nyström (Chen et al. 2011), large-scale clustering (LSC) (Chen and Cai 2011), large-scale multi-view spectral clustering (Li et al. 2015) have been proposed to reduce the high computation of spectral clustering.

In contrast, k-means clustering has been more often applied to large-scale clustering because of its simplicity and general applicability. Two steps are employed in each iteration: updating the cluster centers, and updating the assignments of each point. The computation cost of k-means in each iteration is $\mathcal{O}(nkd)$, where n, k, d are the size of the dataset, the number of clusters, and the dimensionality, respectively. For such large values, even a single iteration is very slow. For example, we show in the experiment on MINIST8M dataset where $n = 8.1$M, $d = 784$, $k = 1000$, k-means takes around 6500s to update in each iteration. In addition, 50.80G is needed to store this dataset. Basically, it is very challenging to directly apply k-means over this scale of dataset in a single machine. Several variants (Elkan 2003; Arthur and Vassilvitskii 2007; Hamerly 2010; Drake and Hamerly 2012; Ding et al. 2015; Bachem et al. 2016) of k-means have been proposed to improve the clustering efficiency. They can decrease the number of iterations, but the running time of each iteration and memory usage are unchanged. Therefore, two main challenges remain to be solved in large-scale clustering: 1) how to reduce the storage of huge data, and 2) how to reduce the computational cost of the clustering methods.

Binary code learning (Wang et al. 2016) has gained increased interests in many large-scale applications. The basic idea of binary code learning is to encode the original high-dimensional data into a set of short binary codes with similarity preservation. The advantage of binary coding is that it can perform an effective search in Hamming space at very low cost of both storage and computation. Many binary code learning methods (Gionis et al. 1999; Gong and Lazebnik 2011; Norouzi, Fleet, and Salakhutdinov 2012; Zhou et al. 2016; Song, Liu, and Meyer 2016; Shen et al. 2017) have been developed, all of which are proposed to facilitate large-scale retrieval and classification, instead of clustering. A pioneering work (Gong et al. 2015) to perform clustering over binary codes was recently proposed. This is a naive two-step approach, which generates

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binary codes and performs clustering separately. Apparently, the binary codes may not be optimal for clustering in this two-step approach, and we show in our experiments that it performs poorly on some datasets. To the best of our knowledge, learning binary codes for clustering has been less well studied and remains a very challenging area.

Inspired by the great success of binary code learning, we propose a novel compressed k-means (CKM) for large-scale clustering. CKM aims to simultaneously learn binary codes and clusters. The advantages of CKM over conventional clustering methods lie in the low cost of computation and storage. Taking the MINIST8M dataset as an example, CKM reduces the storage around 392 times from 50.80G to 129.60M; meanwhile, the running time of CKM in one iteration is 25s, which is nearly 260 times faster than conventional k-means. The main contributions of this work are summarized below:

- We propose a novel binary coding based clustering method, named compressed k-means (CKM), which compresses high-dimensional data into short binary codes. CKM can be applied to large-scale clustering at low computational and storage costs.
- The proposed CKM is formulated to jointly perform binary coding function learning and clustering, such that the learned binary codes are optimal for clustering. Inspired by the recent advances in structural prediction (Yu and Joachims 2009; Norouzi, Fleet, and Salakhutdinov 2012), an upper bound of the empirical loss of the optimization algorithm is presented, for which an efficient optimization algorithm is devised.
- Extensive experiments on four large-scale datasets, demonstrate that the proposed CKM is faster and has lower memory usage than the state-of-the-art large-scale clustering methods.

Notations and Background

Given a dataset $\mathcal{X} = \{\mathbf{x}_i \in \mathbb{R}^d\}_{i=1}^n$, we can write $\mathbf{X} = [\mathbf{x}_1, \ldots, \mathbf{x}_n]$, and the goal of clustering is to group the data points $\{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ into k clusters $\{\mathcal{C}_j\}_{j=1}^k$, such that similar data points can be grouped together. We use the partition matrix $\mathbf{G} = [\mathbf{g}_1, \ldots, \mathbf{g}_n] \in \{0,1\}^{k\times n}$ to represent the clustering results. Let $g_{ij} = 1$ if $\mathbf{x}_i$ belongs to cluster $\mathcal{C}_j$ and $g_{ij} = 0$ otherwise; we call $\mathbf{G}$ the cluster indicator matrix because each column, i.e., $\mathbf{g}_i$ $(1 \le i \le n)$, has one and only one element equal to 1 to indicate the cluster membership, while the remaining elements are 0. We denote the set of such indicator matrices as Ψ.

The k-means method is the most popular clustering method because of its simplicity. It has been identified as one of the top 10 algorithms in data mining (Wu et al. 2008). Formally, k-means aims to minimize the following objective function:

$$\begin{aligned} \min_{\mathbf{G},\mathcal{C}} \quad & \sum_{j=1}^{k}\sum_{\mathbf{x}_i\in\mathcal{C}_j} \|\mathbf{x}_i - \mathbf{c}_j\|^2 = \sum_{j=1}^{k}\sum_{i=1}^{n} g_{ij}\|\mathbf{x}_i - \mathbf{c}_j\|^2 \\ \text{s.t.} \quad & \mathbf{G} \in \Psi^{k\times n} \end{aligned} \tag{1}$$

where $\|\cdot\|$ denotes ℓ_2 norm of a vector, and $\mathbf{c}_j$ is the j-th centroid of the dataset. Because $\mathbf{G} \in \Psi$ is a cluster indicator matrix, k-means is a combinatorial optimization problem that is generally difficult to resolve.

A simple yet popular algorithm for finding a local optimum of the k-means problem starts with a random set of k centers and is as follows: each data point is repeatedly assigned to its nearest center, and the centers are recomputed given the point assignments. This local search, called *Lloyd's* iteration, continues until a stable set of centers is obtained. In each iteration, k-means requires the time complexity of $\mathcal{O}(nkd)$. For a large-scale dataset in which both n and k are large, k-means will be computationally expensive even with medium-length d. It is also very challenging to store the whole dataset and cluster centers in a single machine. Generally, directly applying k-means on a large-scale dataset is inefficient.

A challenging problem naturally raises how to efficiently perform k-means on large-scale datasets. In the following sections, we introduce the binary coding technique to address this issue.

Compressed K-means

Problem Formulation

Given the data matrix $\mathbf{X} \in \mathbb{R}^{d\times n}$, we aim to learn a mapping $b(\mathbf{x})$ that projects d-dimensional real-valued input $\mathbf{x} \in \mathbb{R}^d$ onto a r-dimensional binary code $\mathbf{h} \in \mathcal{H} \equiv \{-1,1\}^r$, where k-means clustering can be efficiently performed. The mapping, referred to as binary coding function, is defined as:

$$b(\mathbf{x};\mathbf{W}) = \text{sign}(f(\mathbf{x},\mathbf{W})) \tag{2}$$

where $\text{sign}(\cdot)$ is the element-wise sign function, and $f(\mathbf{x},\mathbf{W}) : \mathbb{R}^d \to \mathbb{R}^r$ is a real-valued transformation, where $\mathbf{W} \in \mathbb{R}^{d\times r}$. A variety of mathematical forms of f can be used for domain specific practical applications. In this work, we consider a linear transformation $f(\mathbf{x}) = \mathbf{W}^\top\mathbf{x}$ for its simplicity.

The distance between binary codes $\mathbf{h}, \mathbf{e} \in \mathcal{H}$ can be denoted as:

$$\rho_H(\mathbf{h},\mathbf{e}) = \|\mathbf{h} - \mathbf{e}\|^2 \tag{3}$$

For k-means clustering in the Hamming space, we define the loss function of the i-th data point:

$$\begin{aligned} \ell(\mathbf{x}_i) &= \sum_{j=1}^{k} g_{ij}\rho_H(b(\mathbf{x}_i;\mathbf{W}),\mathbf{c}_j) \\ &= \rho_H(b(\mathbf{x}_i;\mathbf{W}),\mathbf{C}\mathbf{g}_i) \end{aligned} \tag{4}$$

where $\mathbf{C} = [\mathbf{c}_1, \ldots, \mathbf{c}_k] \in \{-1,1\}^{r\times k}$. Thus the objective function of the proposed compressed k-means (CKM) is defined as:

$$\begin{aligned} \min \mathcal{L}(\mathbf{W},\mathbf{C},\mathbf{G}) &= \sum_{i=1}^{n}\ell(\mathbf{x}_i) = \sum_{i=1}^{n}\rho_H(b(\mathbf{x}_i;\mathbf{W}),\mathbf{C}\mathbf{g}_i) \\ &= \sum_{i=1}^{n}\|b(\mathbf{x}_i;\mathbf{W}) - \mathbf{C}\mathbf{g}_i\|^2 \\ \text{s.t.} \quad & \|\mathbf{w}_j\| \le \nu, \forall j \in \{1,\ldots,k\}, \text{and} \\ & \mathbf{C} \in \{-1,1\}^{r\times k}, \mathbf{G} \in \Psi^{k\times n} \end{aligned} \tag{5}$$

where $\nu \in \mathbb{R}^+$ is a positive regularization parameter that is used to constrain the scale of $\mathbf{W}$. This is because the scale of $\mathbf{W}$ does not affect the objective function value. We impose the binary constraints on the cluster centers $\mathbf{C}$. In constrst to the conventional k-means, the data points and cluster centers are both hashed into binary codes, which enables us to perform fast distance calculation in clustering.

Direct global optimization of $\mathcal{L}$ is challenging because 1) the objective function is highly non-convex; 2) $b(\mathbf{x}; \mathbf{W})$ is a discrete mapping. In the following section, we will present the technique to address these difficulties.

Upper Bound on Empirical Loss

Inspired by latent structural SVMs (Yu and Joachims 2009; Liu and Tsang 2015), we develop the optimization technique to optimize an upper bound of $\mathcal{L}$. We first re-express the binary coding function as a form of structured prediction (Norouzi, Fleet, and Salakhutdinov 2012):

$$\begin{aligned} b(\mathbf{x}; \mathbf{W}) &= \operatorname{sign}(f(\mathbf{x}; \mathbf{W})) \\ &= \arg\max_{\mathbf{h} \in \mathcal{H}} \ \mathbf{h}^\top f(\mathbf{x}; \mathbf{W}) \\ &= \arg\max_{\mathbf{h} \in \mathcal{H}} \ \mathbf{h}^\top \mathbf{W}^\top \mathbf{x} \end{aligned} \tag{6}$$

Here, (6) holds because that the optimal code should be +1 for the positive entries of $\mathbf{W}^\top \mathbf{x}$, and -1 otherwise.

Based on the structure prediction form of binary coding function, we present a theorem on the upper bound of the loss function of the i-th data point.

Theorem 1. *For arbitrary $\alpha > 0$, the loss function of the i-th data point, i.e., $\ell(\mathbf{x}_i)$, is upper bounded by:*

$$\begin{aligned} \ell(\mathbf{x}_i) \leq \max_{\mathbf{e}_i \in \mathcal{H}} \left(\rho_H(\mathbf{e}_i, \mathbf{C}\mathbf{g}_i) + \alpha \mathbf{e}_i^\top f(\mathbf{x}_i; \mathbf{W}) \right) \\ - \alpha \max_{\mathbf{h}_i \in \mathcal{H}} \left(\mathbf{h}_i^\top f(\mathbf{x}_i; \mathbf{W}) \right) \end{aligned} \tag{7}$$

Proof. This upper bound is easily derived via structural SVM. □

Based on Theorem 1, we can obtain the following *surrogate* objective function:

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{C}, \mathbf{G}} \ & \sum_{i=1}^{n} \Big(\max_{\mathbf{e}_i \in \mathcal{H}} \left(\|\mathbf{e}_i - \mathbf{C}\mathbf{g}_i\|^2 + \alpha \mathbf{e}_i^\top \mathbf{W}^\top \mathbf{x}_i \right) \\ & - \alpha \max_{\mathbf{h}_i \in \mathcal{H}} \left(\mathbf{h}_i^\top \mathbf{W}^\top \mathbf{x}_i \right) \Big) \\ \text{s.t.} \ & \|\mathbf{w}_j\| \leq \nu, \forall j \in \{1, \ldots, k\}, \text{and} \\ & \mathbf{C} \in \{-1, 1\}^{r \times k}, \mathbf{G} \in \Psi^{k \times n} \end{aligned} \tag{8}$$

Optimization

Loss-augmented Inference. To evaluate and use the surrogate objective in (8) for optimization, we must solve a *loss-augmented inference* problem to find the binary code that maximizes the sum of the score and loss term:

$$\begin{aligned} \max_{\mathbf{e}_i} \ & \|\mathbf{e}_i - \mathbf{C}\mathbf{g}_i\|^2 + \alpha \mathbf{e}_i^\top \mathbf{W}^\top \mathbf{x}_i \\ \text{s.t.} \ & \mathbf{e}_i \in \{-1, 1\}^{r \times 1} \end{aligned} \tag{9}$$

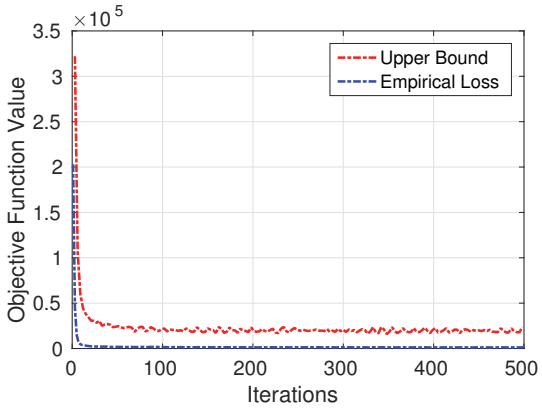


Figure 1: The upper bound and empirical loss with respect to different iterations on RCV1 dataset.

With simple matrix transformations, the solution to $\mathbf{e}_i$ can easily be obtained:

$$\mathbf{e}_i = \operatorname{sign}\left(-2\mathbf{C}\mathbf{g}_i + \alpha \mathbf{W}^\top \mathbf{x}_i\right) \tag{10}$$

Cluster Learning. We next optimize the sub-objective function of clustering in the Hamming space. The sub-objective function with respect to $\mathbf{C}, \mathbf{G}$ is as follows:

$$\begin{aligned} \min_{\mathbf{C}, \mathbf{G}} \ & \sum_{i=1}^{n} \|\mathbf{e}_i - \mathbf{C}\mathbf{g}_i\|^2 \\ \text{s.t.} \ & \mathbf{C} \in \{-1, 1\}^{r \times k}, \mathbf{G} \in \Psi^{k \times n} \end{aligned} \tag{11}$$

The optimization of (11) is similar to conventional k-means. To obtain the locally optimal $\{\mathbf{C}, \mathbf{G}\}$, it is necessary to iteratively update one variable while fixing the other variable until convergence. Below we show that, in each iteration, $\{\mathbf{C}, \mathbf{G}\}$ can be solved via the following theorem.

Theorem 2. *In each iteration, $\{\mathbf{c}_j, \mathbf{g}_i\}$ that minimizes the optimization problem in* (11) *is given by:*

$$\mathbf{c}_j = \operatorname{sign}\left(\sum\nolimits_{g_{ij}=1} \mathbf{e}_i \right) \tag{12}$$

$$g_{ij} = \begin{cases} 1 & j = \arg\min_l \|\mathbf{e}_i - \mathbf{c}_l\| \\ 0 & \text{otherwise} \end{cases} \tag{13}$$

where $i = 1, \ldots, n$, $j = 1, \ldots, k$.

Proof. The proof can be easily obtained similar to the conventional k-means. □

Binary Coding Function Learning. Optimizing the objective function with respect to $\mathbf{W}$ is difficult because it is a convex-concave problem. In this work, inspired by (Norouzi, Fleet, and Salakhutdinov 2012), we employ stochastic gradient descent (SGD) to update $\mathbf{W}$. In each iteration, we randomly sample a data point, i.e., $\mathbf{x}$, and then take a step in the direction that decreases the objective function value. The updating rule of $\mathbf{W}$ can be represented as

$$\mathbf{W} = \mathbf{W} - \eta \tilde{\mathbf{x}} (\mathbf{e} - \mathbf{h})^\top \tag{14}$$

Algorithm 1 Compressed k-means

Input: Training set $\mathbf{X} \in \mathbb{R}^{d \times n}$; code length r; cluster number k; parameters α, ν.
Output: $\mathbf{W}$, $\mathbf{C}$, $\mathbf{G}$.

Initialize $\mathbf{W}$ via Locality Sensitive Hashing (LSH);
Initialize $\mathbf{B} = \text{sign}(\mathbf{W}^\top \mathbf{X})$;
Initialize $\mathbf{C}$ by randomly selecting k binary codes;
repeat
    Update $\mathbf{e}_i$ via (10), $i = 1, \ldots, n$;
    Iteratively update $\mathbf{C}$, $\mathbf{G}$ via (12), (13);
    Update $\mathbf{W}$ using (14) on a small batch;
    Project $\mathbf{W}$ back to the feasible region via (15);
until *convergence*

where η is the learning rate, which is set as 0.001 in this work, $\mathbf{h}$, $\mathbf{e}$ are obtained by the loss inference (6), (10), respectively. As there is a norm constraint on $\mathbf{W}$, we need to project $\mathbf{W}$ back to the feasible region, thus we perform the following operation

$$\mathbf{w}_i = \min\left\{1, \sqrt{\nu}/\|\mathbf{w}_i\|\right\} \mathbf{w}_i \tag{15}$$

where $i = 1, \ldots, r$.

In our implementation, we propose a two-stage scheme. We start the optimization algorithm by initializing $\mathbf{W}$ as a random Gaussian matrix by Locality Sensitive Hashing (LSH) (Gionis et al. 1999). In the first stage, we jointly learn the binary coding function and clustering on a randomly selected subset with $n' = \beta n$ data points, where β is the proportion of the selected data points. In the second stage, we perform clustering on the binary codes of the entire dataset. Here the subset selection is used to speed up the binary function learning. We will show in the experiment that it is enough to learn a good binary function on a small subset for large-scale clustering. In addition, we use mini-batches rather than single data point to compute the gradient, and the batch size is set as 128. The detailed optimization procedure of CKM is described in Algorithm 1.

The theoretical convergence of this update rule has been explored (Hazan, Keshet, and McAllester 2010). In this work, we empirically verify that the update rule lowers both the upper bound and the empirical loss, and converges to a local minimum. Fig. 1 shows the curves of the upper bound and the empirical loss, from where we can clearly see that both converge within a few iterations.

Computational Complexity and Memory Usage

The computational complexity of the proposed CKM consists of the following parts. Loss-augmented inference requires $\mathcal{O}(dr)$ for updating each data point. Updating binary coding function requires $\mathcal{O}(drp)$, where p is the mini-batch size. The most time-consuming part lies on cluster learning, which takes $\mathcal{O}(nk)$ Hamming distance calculation for r-bit codes. In constrast, k-means takes $\mathcal{O}(nk)$ Euclidean distance calculation for d-dimensional real-valued vectors. Thus, CKM is more efficient than k-means, especially when $r \ll d$.

Table 1: Statistics of four large-scale datasets.

Datasets	#Sample	#Feature	#Classes
RCV1	193844	1979	103
CovType	581012	54	7
ILSVRC2012	1331167	4096	1000
MNIST8M	8100000	784	10

To calculate memory usage, CKM needs to store the transformation matrix $\mathbf{W}$, which counts for the storage of $\mathcal{O}(rd)$ real-valued numbers. The data points and cluster centroids are stored by CKM at the cost of $\mathcal{O}((n + k)r)$ bits. k-means requires the storage of $\mathcal{O}((n+k)d)$ real-valued numbers. Therefore, CKM has much lower memory cost than k-means.

Experiments

In this section, we evaluate the proposed clustering method on four large-scale datasets. All the computations reported in this study are performed on a Red Hat Enterprise 64-Bit Linux workstation with 18-core Intel Xeon CPU E5-2680 2.80 GHz and 256 GB memory.

Datasets

We conduct experiments on four large-scale datasets, whose statistics are summarized in Table 1.

- **RCV1**[1]: a subset (Chen et al. 2011) of an archive of 804414 manually categorized newswire stories from Reuters Ltd. It has 193844 documents in 103 categories. Following previous studies (Wang et al. 2011a), we remove the keywords (features) appearing less than 100 times in the corpus, which results in 1979 (out of 47236) keywords in our experiment.
- **CovType**[2]: consists of 581012 instances for predicting forest cover type from cartographic variables. Each sample belongs to one of seven types (classes).
- **ILSVRC2012**[3]: a subset of ImageNet (Deng et al. 2009). It contains 1000 object categories and more than 1.2 million images. As in (Lin, Shen, and van den Hengel 2015), we use the 4096-dimensional features extracted by the convolution neural networks (CNN) model (Krizhevsky, Sutskever, and Hinton 2012) to represent the images.
- **MNIST8M**[4]: consists of around 8.1 million images of handwritten digits from 0 to 9. The feature is the same as MNIST dataset: 784-dimensional original pixel values.

Comparison Methods

To demonstrate the effectiveness of the proposed CKM, we compare it with five state-of-the-art large-scale clustering methods, consisting of two k-means methods, two spectral clustering methods, and a naive two-step clustering method

[1] http://alumni.cs.ucsb.edu/∼wychen/sc.html
[2] https://archive.ics.uci.edu/ml/
[3] http://www.image-net.org/challenges/LSVRC/2012/
[4] http://www.csie.ntu.edu.tw/∼cjlin/libsvmtools/datasets/

Table 2: Running time (in seconds) of clustering on four large-scale datasets.

Dataset	k-means		k-means++		Nyström		LSC-K		LSH+bk-means		CKM	
	Time	Speedup	Time	Speedup	Time	Speedup	Time	Speedup	Time	Speedup	Time	Speedup
RCV1	191s	1×	254s	0.75×	61s	3.13×	206s	0.93×	4s	47.75×	16s	11.94×
CovType	17s	1×	11s	1.55×	39s	0.44×	65s	0.26×	1s	17.00×	3s	5.67×
ILSVRC2012	8523s	1×	18469s	0.46×	2626s	3.25×	22173s	0.38×	89s	95.76×	250s	34.09×
MINIST8M	9718s	1×	2578s	3.77×	1418s	6.85×	5107s	1.90×	101s	96.22×	248s	39.19×

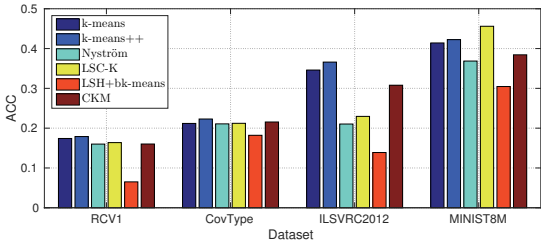


Figure 2: Clustering accuracy (ACC) on four large-scale data sets.

using LSH plus bk-means (Gong et al. 2015). The details of these methods are given below.

- **k-means**: is the conventional k-means method based on Euclidean distance. It can be seen as a baseline method.
- **k-means++** (Arthur and Vassilvitskii 2007): a variant of k-means, which provides a good initialization that is provably close to the optimal solution.
- **Nyström** (Chen et al. 2011): a parallel large-scale spectral clustering method based on Nyström approximation. The code is available online[5], and we choose the Matlab version with orthogonalization.
- **LSC-K** (Chen and Cai 2011): the landmark-based large-scale spectral clustering method using k-means for landmark selection. We download the Matlab code from the authors' website[6].
- **LSH+bk-means** (Gong et al. 2015): first uses Locality Sensitive Hashing (LSH) (Gionis et al. 1999) to generate a random Gaussian matrix, by which data points are hashed into binary codes. bk-means (Gong et al. 2015) is then applied to the generated binary codes for clustering. This naive two-step method can be viewed as a baseline for binary coding based clustering methods.

We empirically set the number of landmarks in LSC-K and Nyström as 500 according to the parameter setting in (Chen and Cai 2011), and the number of neighbors in LSC-K as 6. For the binary coding based methods, the binary code length r is set as 32 for CovType, and 128 for the other three high-dimensional datasets. For the proposed CKM, we empirically set the ratio of the selected subset β as 0.01, parameter α as 10, and ν as 1.

[5]http://alumni.cs.ucsb.edu/∼wychen/sc.html

[6]http://www.cad.zju.edu.cn/home/dengcai/

Table 3: Memory usage of k-means and CKM on four large-scale datasets. 'Mem.' denotes memory usage. 'Red.' denotes the times of memory reduction compared to k-means.

Dataset	k-means		CKM	
	Mem.	Red.	Mem.	Red.
RCV1	3.07GB	1×	3.10MB	988×
CovType	0.25GB	1×	2.32MB	432×
ILSVRC2012	43.62GB	1×	21.30MB	2048×
MINIST8M	50.80GB	1×	129.60MB	392×

Evaluation Metric

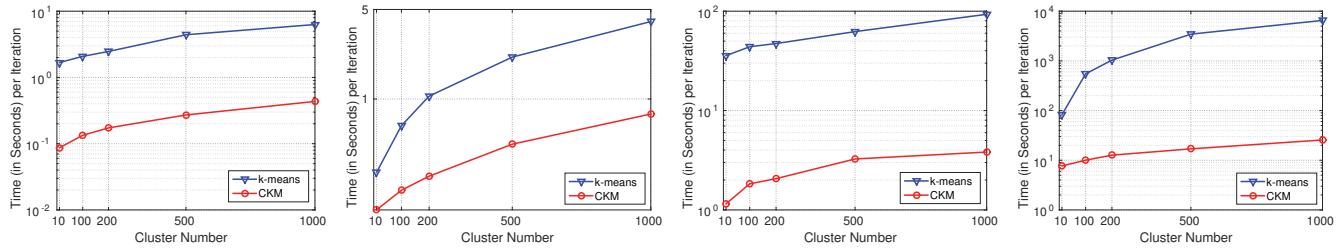
We evaluate clustering quality by Accuracy (Chen and Cai 2011). Given the data point $\mathbf{x}_i$, let o_i and s_i be its resultant clustering label and ground-truth label, respectively. The accuracy is defined as ACC $= \frac{\sum_{i=1}^{n} \delta(s_i, \text{map}(r_i))}{n}$, where $\delta(a, b)$ denotes the delta function that returns 1 if $a = b$ and 0 otherwise, and map(r_i) is the best mapping function for permuting the cluster labels to match the ground-truth labels. A larger ACC value indicates better clustering performance.

In addition, we also conduct the comparisons in terms of computation and memory costs.

Results

Accuracy: The accuracy results of all the methods on four datasets are reported in Fig. 2. We find several interesting points as follows: 1) Among the comparisons, k-means is stable on four datasets, and k-means++ generally outperforms k-means. LSC-K performs best on MINIST8M, but fails to work well on ILSVRC2012. LSC-K performs better than Nyström. 2) The proposed CKM clearly outperforms LSH+bk-means. LSH+bk-means is a naive two-step method, thus the generated binary codes may not be optimal for clustering. The accuracy of LSH+bk-means is very low on RCV1, ILSVRC2012. 3) CKM generally achieves comparable accuracy to the best results.

Time: Table 2 shows the running time of all the methods on four datasets. We can see from this table that 1) LSH+bk-means is the fastest among all the methods. It is faster than CKM, because CKM needs the additional time to learn the binary coding function, while the binary function is LSH is random. 2) The proposed CKM takes the second place. It is more efficient than conventional clustering methods. In particular, CKM is nearly 39 times faster than k-means on MINIST8M. 3) k-means++ is generally faster than k-means on CovType and MINIST8M, but slower than k-means on RCV1 and ILSVRC2012. Among the spectral clustering methods, Nyström is faster than LSC-K.



(a) RCV1 (b) CovType (c) ILSVRC2012 (d) MNIST8M

Figure 3: Running time (in seconds) of k-means and CKM for one iteration on (a) RCV1, (b) CovType, (c) ILSVRC2012, (d) MNIST8M. Y axis is in log scale.

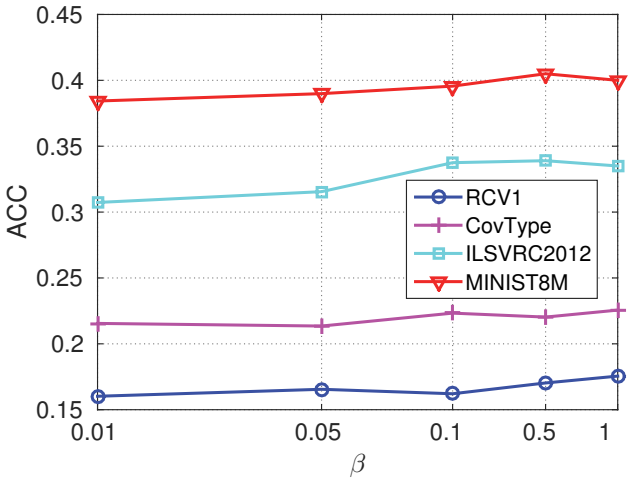


Figure 4: Clustering accuracy with respect to different β. X axis is in log scale.

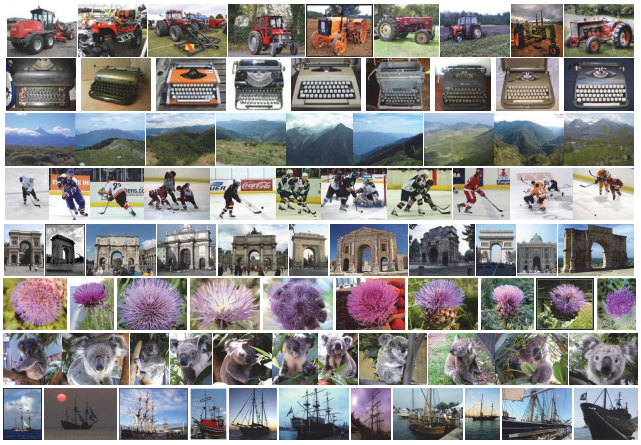


Figure 5: Illustration of cluster samples of ILSVRC2012 dataset generated by the proposed CKM. Each row illustrates several representative images of one cluster.

In addition, we compare the running time of k-means and CKM in one iteration. The running time of the two methods in one iteration with respect to different numbers of clusters is shown in Fig. 3. As can be seen, CKM is clearly much faster than k-means among all the cases. This is because CKM uses Hamming metric for distance calculation, which is more efficient than the conventional Euclidean distance calculation in k-means.

Memory Usage: Table 3 reports the memory usage of k-means and CKM. We clearly observe that compared with k-means, CKM significantly reduce the memory storage of data. Particularly, CKM only needs to store 21.30M of binary codes to represent ILSVRC2012, which is nearly 2048 times memory reduction to k-means. This result implies that CKM can perform clustering over very large-scale dataset in a single machine.

Sensitivity Study: We now provide a more careful analysis of the proposed CKM on the sensitivity to the key parameters in the clustering tasks. The ratio β is ranged from [0.01, 0.05, 0.1, 0.5, 1], and clustering accuracy with respect to different β is shown in Table 4. From Table 4, we observe that the clustering accuracy slightly improves as β increases, that is, β does not heavily influence the clustering performance. This reveals that the binary coding function in CKM is well learned even on a small subset of large-scale datasets. The sensitivtiy results on other paramaters are presented in supplementary materials.

Case Study: We present a case study in which the proposed CKM is applied to a large-scale image clustering application. Fig. 5 shows sample clusters of ILSVRC2012 generated by CKM. Each row illustrates several representative images of one cluster. We observe from this figure that similar images are well clustered. This case study suggests that CKM works well in practical large-scale clustering applications.

Conclusion

This work focuses on the challenging problem of fast clustering over large-scale datasets. We propose a novel compressed k-means (CKM) to generate optimal binary codes for clustering. Compared to existing clustering methods, CKM enjoys both computational and memory efficiency. Extensive experiment results on four large-scale datasets, including two million-scale datasets, suggests that CKM is able to cluster very fast with limited memory, yet achieves

comparable accuracy to the state-of-the-art methods.

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