NNK-MEANS: DICTIONARY LEARNING USING NON-NEGATIVE KERNEL REGRESSION

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ABSTRACT

An increasing number of systems are being designed by first gathering significant amounts of data, and then optimizing the system parameters directly using the obtained data. Often this is done without analyzing the dataset structure. As task complexity, data size, and parameters all increase to millions or even billions, data summarization is becoming a major challenge. In this work, we investigate data summarization via dictionary learning, leveraging the properties of recently introduced non-negative kernel regression (NNK) graphs. Our proposed NNK-Means, unlike competing techniques, such as kSVD, learns geometric dictionaries with atoms that lie in the input data space. Experiments show that summaries using NNK-Means can provide better discrimination compared to linear and kernel versions of kMeans and kSVD. Moreover, NNK-Means has a scalable implementation, with runtime complexity similar to that of kMeans.

Index Terms— Data summarization, cluster analysis, dictionary learning, neighborhood methods, kernel methods.

1. INTRODUCTION

Massive high-dimensional datasets of various modalities are becoming an increasingly common input for system design. While it is increasingly easier to collect these datasets with millions or even billions of points, the methods for exploratory (understanding or characterizing the data) and confirmatory (confirming the validity and stability of a system designed using the data) analysis are not as scalable and require the development of techniques that can cope with big data sizes [1, 2]. Briefly put, data summarization methods aim to represent large datasets by a small set of elements, the insights from which can be used to organize the dataset into clusters, classify observations to its clusters, or detect outliers [3]. These summaries can be obtained for a given class in datasets with label information, but are, in general, decoupled from downstream data-driven system designs and thus different from coresets and sketches [4, 5].

Clustering methods such as kMeans [6], vector quantization [7] and their variants [8], are among the most prevalent approaches to data summarization [9, 10]. A desirable property for summarization, which can be obtained with clustering methods, is the geometric interpretability of elements in the summary. For example, with the kMeans method elements in the summary are centroids, which are obtained by averaging points in the input data space, and thus are themselves in the same data space. Note that in a clustering approach each point in the dataset is a 1-sparse representation based on the nearest cluster center. Consequently, when input data points are interpreted based on a kMeans summary they can only use the attribute (e.g., label) of the nearest neighbor (cluster center). Thus, the constraint of 1-sparsity leads to hard partitioning of the input data space. This suggests that better summaries may be possible if the optimization criterion allows each point in the original space to be approximated by a linear combination of summary points.

Based on this observation, in this paper, we investigate data summarization using a dictionary learning (DL) framework where the summary, or dictionary, is optimized for k-sparse in data representation, with k greater than 1, i.e., each point is represented by a k-sparse combination of elements (atoms) from an adaptively learned set, the dictionary. It is important to note that while DL has witnessed great progress and success in a range of applications, the use of dictionary learning methods for data summarization has not been considered before. In order to design a dictionary with geometry properties resembling those of kMeans, we leverage our work on neighborhood definition with non-negative kernel regression (NNK) [11, 12] and propose a novel NNK-Means dictionary learning technique for data summarization. NNK-Means learns dictionaries optimized for higher sparsity with atoms that belong to the given data manifold as in the kMeans approach. In addition, the runtime of proposed NNK-Means is similar to that of kMeans, and can take advantage of fast neighborhood search tools [13, 14] for scaling to big datasets. The central idea behind NNK-Means involves a combination of sparsity, non-negativity, and kernels. These concepts, though studied individually [15, 16, 17], have neither had a unified investigation nor an algorithmic development with emphasis on dictionary geometry for data summarization.

Note that earlier DL schemes such as the method of optimal directions (MOD) [18] and the kSVD algorithm [19], and its extensions via kernels [20], namely, kernel kSVD [21, 15], are also suitable for DL-based data summarization but their use in practice has some disadvantages. Firstly, DL methods learn atoms optimized to represent data using the entire dictionary [22]. This means that atoms learned are not guaranteed to be points in the input manifold and do not have geometric properties as those of cluster centers in kMeans. Secondly, although DL methods perform well in sparse signal and image representation tasks, they often require additional discrimination-promoting terms such as those in [23, 24, 25] for use in machine learning problems. Finally, current DL schemes are not scalable and are impractical even for datasets of modest size [26, 27].

Our experiments show that the proposed NNK-Means DL i) selects elements in the data space for summarization, ii) outperforms other DL methods in terms of downstream classification using class-specific summaries on USPS, MNIST, and CIFAR10, and iii) achieves train and test runtimes similar to kernel kMeans, and $O(T \times \text{vec})$ and $7 \times$ faster than kernel kSVD.

2. PROBLEM SETUP AND BACKGROUND

Sparse Dictionary Learning: Given a dataset of $N$ data points represented by matrix $X \in \mathbb{R}^{d \times N}$, the goal of DL is to find a dicti-
**Fig. 1:** Left: Proposed NNK-Means. The algorithm alternates between sparse coding ($\mathbf{W}$) using NNK and dictionary update via $\mathbf{A}$ until either the dictionary elements converge, or a given number of iteration/reconstruction error is achieved. Middle: During sparse coding, a kMeans approach assigns each data point to its nearest neighbor while NNK represents each data point in an adaptively formed convex polytope made of the dictionary atoms. Right: Comparative summary between dictionary learning methods and proposed NNK-Means approach. A kMeans approach offers a 1-sparse dictionary learning approach while a kSVD offers a more general approach where the sparse coding stage accommodates for a chosen, fixed $k_0$-sparsity. The assignment in kSVD does not constrain the coding weights to be non-negative and lacks a geometric interpretation. NNK-Means has adaptive sparsity that relies on the geometry of atoms around each data to be represented.

A straightforward way of kernelizing DL would involve replacing the input data by their respective Reproducing Kernel Hilbert Space (RKHS) representation. However, such a setup is unable to leverage the kernel trick [29, 30] and thus to overcome this problem, [21] suggest decomposing the dictionary and solving a modified objective (1), namely,

$$
\mathbf{A}, \mathbf{W} = \arg \min_{\mathbf{A}, \mathbf{W}} \sum_{i=1}^{N} \| \mathbf{X}_i - \mathbf{D} \mathbf{W}_i \|_F^2
$$

where the $\ell_0$ constraint on $\mathbf{W}$ corresponds to the sparsity requirements on the columns of the reconstruction coefficients $\mathbf{W}_i \in \mathbb{R}^M$ and $\| \cdot \|_F$ represents the Frobenius norm of the reconstruction error associated with the representation. The solution to (1) in MOD or kSVD is found in an iterative manner alternating between sparse coding ($\mathbf{W}$) and dictionary update steps ($\mathbf{D}$).

A kMeans algorithm can be written as objective (1) with 1-sparsity constraint on the sparse coding step, i.e., each column of $\mathbf{W}$ is constrained to have only one nonzero value. Soft variants of kMeans or mixture model learning using expectation maximization (EM) [28] can be considered DL models where this sparsity constraint is removed and one gets to use all columns of $\mathbf{D}$. These similarities only provide a partial picture and differences do exist: First, the coefficients involved in the sparse coding step of kMeans, both the hard and soft cluster variants, are non-negative. Secondly, in kMeans, sparse coding of data is done by considering the proximity of the dictionary elements to the data, whereas in kSVD or MOD, the coding is done by searching for atoms that maximally correlate with the residual. Finally, the dictionary updates associated in these methods are not the same and lead to different dictionaries. A straightforward way of kernelizing DL would involve replacing the input data by their respective Reproducing Kernel Hilbert Space (RKHS) representation. However, such a setup is unable to leverage the kernel trick [29, 30] and thus to overcome this problem, [21] suggest decomposing the dictionary and solving a modified objective (1), namely,

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$$

where $\mathbf{X} = \phi(\mathbf{X})$ corresponds to a non-linear mapping of the data into a high, possibly infinite, dimensional space. In this setup, one learns a dictionary ($\mathbf{D} = \Phi \mathbf{A}$) via the coefficient matrix $\mathbf{A} \in \mathbb{R}^{N \times M}$. This formulation is similar to kMeans [6, 31] where the atoms are obtained via positive weighted averaging of the input data.

**Non-Negative Kernel Regression:** The starting point for our DL method is our graph construction framework using non-negative kernel regression (NNK) [11, 12]. NNK formulates neighborhoods as a signal representation problem, where each data point (represented as a function in RKHS) is to be approximated by functions corresponding to its neighboring points, i.e.,

$$
\min_{\theta \geq 0} \| \phi(x_i) - \Phi \theta \|_2^2,
$$

where $\Phi_e$ contains the RKHS representation of a pre-selected set of data points that are good candidates for NNK neighborhood. Unlike k-nearest neighbor or $\epsilon$-neighborhood, where a neighbor is selected based on only $\phi(x_i)$ or $\phi(x_j)$, and can be viewed as representation using thresholding, NNK leads to an improved and robust neighborhoods, that avoids selecting two neighbors that are similar to each other. Geometrically, this can be explained using hyperplanes, one per selected NNK neighbor, which applied inductively leads to a convex polytope around the data such as the one in Figure 1.

**3. PROPOSED METHOD: NNK-MEANS**

We present a data summarization approach using DL that draws ideas from kMeans and our work on NNK neighborhood [11]. We propose a two-stage learning scheme where we iteratively solve sparse coding and dictionary update until convergence, or until a predefined number of iteration or reconstruction error is reached. We describe the two steps, the respective optimization involved, interpretation, and runtime complexity in this section.

**Sparse Coding:** In this stage, the dictionary representation, here $\mathbf{A}$, is assumed to be fixed. Given a dictionary, in this step we seek to find a sparse matrix $\mathbf{W}$ that optimizes data reconstruction in kernel space. We will additionally require the coefficients of representation to be non-negative with the number of nonzero coefficients at most $k$. Thus, the objective to minimize at this step is

$$
\mathbf{W} = \arg \min_{\mathbf{W} \geq 0} \| \Phi - \Phi \mathbf{A} \mathbf{W} \|_F^2
$$

where $\Phi_i$ corresponds to the RKHS representation of data $x_i$. Solving for each $\mathbf{W}_i$ in equation (4) involves working with a $N \times N$ kernel matrix leading to run times that scale poorly with the size of the dataset. However, the geometric understanding of the above non-negative kernel regression objective in [11], allows us to efficiently solve for the sparse coefficients ($\mathbf{W}_i$) for each data point by selecting and working with a smaller subset of data points. Objective (4)
can be rewritten for each input data point as
\[ \hat{\theta}_i = \arg \min_{\theta \geq 0} \| \phi_i - \Phi A \theta \|_2^2 \] (5)
\[ \implies \hat{W}_{i,S} = \hat{\theta}_i, \quad \hat{W}_{i,S^c} = 0 \]
where the set \( S \) corresponds to the selected subset of indices, here the \( k \)-nearest neighbors, corresponding to the set of the dictionary atoms \( \Phi A \) that can have a nonzero influence in the sparse non-negative reconstruction. The above reduced objective can be solved efficiently as in NNK graphs [11]. Further, due to the adaptivity of NNK to the relative position of the atoms in the neighborhood of the data, the number of NNK neighbors saturates to a constant and thus one can choose to remove the explicit constrain on the sparsity by choosing a large enough subset \( S \). The geometric nature of NNK allows us to explain the sparse coding step, leverage similarity search methods for scaling to large datasets, and provide interpretation to the obtained solution, very much similar to kMeans, where each data is represented by a set of neighbors rather than just 1. The complexity analysis of this step comprises of a neighborhood search \( O(NMd) \) and a non-negative quadratic optimization of \( O(Nk^3) \) runtime.

**Dictionary Update:** For this stage, we will assume the sparse codes for each training data, namely \( W \), are calculated and fixed. Thus, the requirement for this stage is to update \( A \) such that the reconstruction error is minimized. Here, we propose an update similar to MOD, where the dictionary matrix \( A \) is obtained based on \( W \) as
\[ \hat{A} = W^T (WW^T)^{-1} \] (6)
The runtime associated with this step is \( O(M^3 + NkM) \), where we use the fact that \( W \) has at most \( Nk \) non zero elements. We note that using \( k \)-nearest neighbor directly for sparse coding, apart from lacking adaptivity, leads to instabilities at the dictionary update stage and thus is unsuitable for DL in a similar setup.

**Proposition 1.** The dictionary update rule in equation (6) reduces to kMeans dictionary update \( A = W^T \Sigma^{-1} \) when \( W = N \) columns from \( (e_1 \ldots e_M) \), where \( e_m \) is a basis vector, i.e., \( e_m = 0 \) \( \forall i \neq m \) and \( e_{mn} = 1 \) and \( \Sigma \in \mathbb{R}^{N \times M} \) is a diagonal matrix containing the degree or number of times each basis vector \( e_m \) appears in \( W \).

**Algorithm 1:** NNK-Means Algorithm

| Input : Data \( X \in \mathbb{R}^{d \times N} \), Kernel \( \kappa(x,y) \in [0,1] \), Max. sparsity \( k \), Max. iteration \( T \), Tolerance \( \xi \) |
| Initialize : Set \( A \) to select \( M \) random points of input data |
| for \( t = 1, 2, \ldots T \) do |
| \( i = 1, 2, \ldots N \) do |
| \( S = \{ k \) nearest neighbors of node \( i \) in dictionary\} |
| \( \theta_S = \min_{\theta \geq 0} \frac{1}{2} \theta^T K_{S,S} \theta - K_{S,i}^T \theta \) |
| \( E_i = 1 - 2K_{S,i} \theta_S + \theta_S^T K_{S,S} \theta_S \) |
| \( W_{i,S} = \theta_S, \quad W_{i,S^c} = 0 \) |
| if \( \sum_{i=1}^{N} E_i \leq N \xi \) then |
| break // reconstruction error small |
| end |
| Output : Dictionary matrix \( A \), Sparse Code \( W \) |

4. EXPERIMENTS

We study the effectiveness of proposed NNK-Means approach for data summarization using DL and evaluate the obtained dictionaries.
in a sparse representation based classification. Note that learning a good summary corresponds to being able to discriminate and classify test queries better. This experiment setup is the same as that used in [21] and [27] and involves learning a dictionary \( \{ A_i \}_{i=1}^C \) for each class in training data with classification done based on the class specific reconstruction error \( \{ e_i \}_{i=1}^C \), i.e., we sparse code the query \( x_q \) using each dictionary \( A_i \), and assign the query to the class \( (c) \) with lowest reconstruction error \( (c) \). We first present a synthetic example to demonstrate the similarities and differences in each approach and then asses the performance in a more realistic scenario with USPS [32], MNIST [33], and CIFAR10 [34] datasets. We show gains in classification using NNK-Means and compare it to that obtained with kMeans, kSVD, and their kernelized versions. We also compare the train and test runtime of each DL method with that of ours and show that proposed NNK-Means results in better classification with adaptive sparsity of representations at a scalable training and test run times. For sparse coding and DL we use the efficient implementations from omp-box and kSVD-box libraries [35] and Kernel kSVD code of [21] as in [27]. We use a Gaussian kernel \( \kappa(x,y) = \exp(||x-y||^2/2\sigma^2) \) with \( \sigma = 1 \) in all experiments.

Synthetic dataset: We consider a 4-class dataset consisting of samples generated from a non-linear manifold and corrupted with gaussian noise. The first plot in Figure 2 shows the training data and test data used for the experiment with their corresponding labels. Since the data corresponding to each class have the same support, namely the entire \( \mathbb{R}^d \), dictionaries learned using kSVD are indistinguishable for each class and leads to at chance performance in classification of test queries. On the contrary, a kernelized version of kSVD is better able to handle the manifold, though non-robust at some test locations, at the cost of increased computational complexity. We see that a non-negative sparse coding is able to handle input non-linearity even when constrained to 1-sparsity (kMeans).

**USPS, MNIST, CIFAR10:** We demonstrate the performance of our method to summarize high dimensional data in a more practical setting with USPS, MNIST and CIFAR10 datasets. We use as features the image pixel values for USPS and MNIST dataset. For CIFAR10, we train a self-supervised learning model using SimCLR loss [36] on unlabelled training data for extracting features for our experiment. We use the standard training/testing split for each dataset and standardize the feature vectors of each dataset to zero mean and variance one. We also report here results of DL with a subset of the training dataset, namely MNIST-S and CIFAR10-S, for a fair comparison with kernel kSVD. We note that the kernel versions of kSVD using entire training dataset of MNIST and CIFAR10 timed out due to computational constrain. Reported results are the average over 10 runs. Table 1 shows overall classification accuracy of various methods on presented datasets. It is evident that proposed NNK-Means is able to efficiently and quickly learn a compact set of atoms that are capable of representing each class which in turn leads to better classification of test queries as can be seen in Figure 3.

**Table 1:** Classification accuracy (in %, higher is better) on MNIST and CIFAR10 dataset and their subset (S, 20% of randomly sampled training set). Each method learns a 50 atom dictionary for each class, initialized randomly, with maximum sparsity constraint, where applicable, of 30 and run for at most 10 iterations. NNK-Means consistently produces better classification in terms of test accuracy while having a reduced runtime in comparison to kSVD approaches and comparable to that of kernel kMeans. Kernel k-SVD produces comparable performance but at the cost of runtime, about \( 67 \times \) and \( 7 \times \) slower train and test time relative to NNK-Means.

**5. CONCLUSION**

We investigate DL methods for data summarization and propose an improved framework, NNK-Means, that can adaptively represent data using a sparse combination of summary elements. NNK-Means learns atoms that are geometric like kMeans centroids and leverages neighborhood tools to efficiently perform sparse coding with a selected subset of atoms. Experiments show that our method has runtimes similar to kernel kMeans while learning dictionaries that can provide better discrimination than competing methods. In the future, we plan to study the trade-offs associated with summary size and the use of obtained summaries in improving system analysis and design.
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