GRAPH REGULARIZED TENSOR TRAIN DECOMPOSITION

Seyyid Emre Sofuoglu and Selin Aviyente

Department of Electrical and Computer Engineering, Michigan State University, East Lansing, MI.

1. INTRODUCTION

With the advances in data acquisition technology, tensor objects are collected in a variety of applications including multimedia, medical and hyperspectral imaging. As the dimensionality of tensor objects is usually very high, dimensionality reduction is an important problem. Most of the current tensor dimensionality reduction methods rely on finding low-rank linear representations using different generative models. However, it is well-known that high-dimensional data often reside in a low-dimensional manifold. Therefore, it is important to find a compact representation, which uncovers the low-dimensional tensor structure while respecting the intrinsic geometry.

In this paper, we propose a graph regularized tensor train (GRTT) decomposition that learns a low-rank tensor train model that preserves the local relationships between tensor samples. The proposed method is formulated as a nonconvex optimization problem on the Stiefel manifold and an efficient algorithm is proposed to solve it. The proposed method is compared to existing tensor based dimensionality reduction methods as well as tensor manifold embedding methods for unsupervised learning applications.

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2.2. Tensor-Train Decomposition

Using MPS, each element of $\mathcal{Y}_t$ can be represented as [15]:

$$\mathcal{Y}_t(i_1, i_2, \ldots, i_N) = \mathcal{U}_1(i_1, i_2) \mathcal{U}_2(i_2, i_3, \ldots) \mathcal{U}_k(i_k, \ldots) \mathcal{X}_{i_1, i_2+1, \ldots, i_N, i_{N+1, \ldots}} \mathcal{U}.$$  

(2)

where $\mathcal{U}_n \in \mathbb{R}^{r_{n-1} \times r_n \times r_{n+1}}$ for $n \leq k$, $\mathcal{U}_n \in \mathbb{R}^{r_n \times r_{n+1}}$ for $n > k$ are the tensor factors, $r_n < l_n, \forall n \in \{1, \ldots, N\}$ and correspond to the ranks of the different modes. $\mathcal{X} \in \mathbb{R}^{r_{k+1} \times \ldots \times r_N}$ is the low dimensional projection matrix. The parameter $k$ is selected using a center of mass approach to reduce computational complexity, i.e. $k$ is selected such that $\prod_{n=1}^{N} l_n - \prod_{n=k+1}^{N} l_n$ is minimized. TT decomposition given in [2] can be rewritten as, $\mathcal{Y}_t = \mathcal{U}_1 \times_1 \mathcal{X}_2 \times_2 \mathcal{U}_3 \times_3 \ldots \mathcal{X}_N \times_N \mathcal{U}_N$ [14].

When $\mathcal{Y}_t$ is reshaped into a matrix, [2] can be equivalently expressed as a matrix projection $T_k(\mathcal{Y}_t) = [\mathcal{U}_n \odot U_{n,k}] X_{r_{k+1}}$, where $U_{n,k} = \mathcal{U}_1 \mathcal{U}_2 \ldots \mathcal{U}_k$ is the $n$th right singular subspace of $\mathcal{U}_1 \times_1 \mathcal{X}_2 \times_2 \mathcal{U}_3 \times_3 \ldots \mathcal{U}_k \times_k \mathcal{X}_{k+1}$ for $n \leq k$ left orthogonal, $U_{n,k}$ is also left orthogonal [13]. Similarly, when $\mathcal{R}(U_{n,k})$ for $n > k$ are right orthogonal, $U_{n,k}$ is right orthogonal.

3. GRAPH REGULARIZED TENSOR-TRAIN

Our goal is to find a TT projection such that the geometric structure of the samples $\mathcal{Y}_t$ is preserved, i.e. the distance between the samples, $\mathcal{Y}_t$, should be similar to that between the projections $X_t$, while the reconstruction error of the low-rank TT decomposition is minimized.

This goal can be formulated through the following cost function as:

$$f_O(\{\mathcal{U}\}, \mathcal{X}) = \sum_{s=1}^{S} \left\| Y_s - U_1 \times_1 \ldots \times N U_N \right\|^2_F + \lambda \sum_{s=1}^{S} \sum_{s' \neq s} \left\| X_s - X_{s'} \right\|^2_F w_{ss'}, \quad \mathcal{L}(U) = \| u_in \|, \forall n,$$

where $\{\mathcal{U}\}$ denotes the set of tensor factors $\mathcal{U}_n, \forall n \in \{1, \ldots, N\}$, $\mathcal{X} \in \mathbb{R}^{r_{k+1} \times \ldots \times r_N}$ is the tensor whose slices are $X_n$ and $w_{ss'}$ is the similarity between tensor samples defined by:

$$w_{ss'} = \begin{cases} 1, & \text{if } \mathcal{Y}_s \in N_k(\mathcal{Y}_{s'}) \text{ or } \mathcal{Y}_{s'} \in N_k(\mathcal{Y}_s), \\ 0, & \text{otherwise} \end{cases},$$

(3)

where $N_k(\mathcal{Y}_s)$ is the k-nearest neighborhood of $\mathcal{Y}_s$.

The objective function can equivalently be expressed as:

$$f_O(\{\mathcal{U}\}, \mathcal{X}) = \left\| \mathcal{X} - L^{\mathcal{U}_1} \times_1 \ldots \times N L^{\mathcal{U}_N} \right\|^2_F + \lambda tr \left( X^T L \times_1 X \right),$$

where $\mathcal{X}$ is the permutated version of $\mathcal{Y}_t$ such that the last mode is moved to the $(k+1)$th mode and all modes larger than $k$ are shifted by one mode, $W \in \mathbb{R}^{r_{k+1} \times \ldots \times r_{N}}$ is the adjacency matrix and $L = D - W \in \mathbb{R}^{S \times S}$ is the graph Laplacian where $D$ is a diagonal degree matrix with, $D_{ss} = \sum_{s=1}^{S} w_{ss'}$.

3.1. Optimization

The goal of obtaining low-rank tensor train projections that preserve the data geometry can be achieved by minimizing the objective function as follows:

$$\arg\min_{\{\mathcal{U}\}} f_O(\{\mathcal{U}\}, \mathcal{X}), \text{ s.t. } L(U) \mathcal{L}(U) = I_{r_n}, \quad \text{for } n \leq k, \quad \text{and } R(U) \mathcal{R}(U) = I_{r_n}, \quad \text{for } n > k.$$

As we want our tensor factors to be orthogonal, the solutions lie in the Stiefel manifold $S_{r_n}$, i.e. $\mathcal{L}(U_n) \in S_{r_n}$ for $n \leq k$ and $\mathcal{R}(U_n)^T \in S_{r_n}$ for $n > k$. Although the function $f_O()$ is convex, the optimization problem is nonconvex due to the manifold constraints on $U_n$. The solution to the optimization problem can be obtained by Alternating Direction Method of Multipliers (ADMM). In order to solve the optimization problem we define $\{V\}$, as the set of auxiliary variables $V_n, \forall n \in \{1, \ldots, N\}$ and rewrite the objective function as:

$$\arg\min_{\{\mathcal{V}\}} f_O(\{\mathcal{V}\}) \quad \text{subject to } \mathcal{U}_n = \mathcal{V}_n, \forall n \in \{1, \ldots, N\}.$$  

The partial augmented Lagrangian is given by:

$$\mathcal{L}(\{\mathcal{U}\}, \{\mathcal{V}\}) = f_O(\{\mathcal{V}\}) - \sum_{n=1}^{N} \left( Z_n \times_1 Z_n \times_2 \ldots \times_3 (V_n - U_n) + \frac{\gamma}{2} \| V_n - U_n \|^2_F \right),$$

where $Z_n$ are the Lagrange multipliers and $\gamma$ is the penalty parameter.

As each tensor factor is independent from the others, we update the variables for each mode $n$ using the corresponding part of the augmented Lagrangian:

$$\mathcal{L}_n(\mathcal{U}_n, \mathcal{V}_n, Z_n) = f_O(\mathcal{V}_n) - Z_n \times_1 Z_n \times_2 \ldots \times_3 (V_n - U_n) + \frac{\gamma}{2} \| V_n - U_n \|^2_F,$$

where $f_O(\mathcal{V}_n)$ denotes the objective function where all variables other than $\mathcal{V}_n$ are fixed. The solution for each variable at iteration $t + 1$ can then be found using a step-by-step approach as:

$$V_n^{t+1} = \arg\min_{\mathcal{V}_n} \mathcal{L}_n(\mathcal{U}_n, \mathcal{V}_n, Z_n),$$

$$U_n^{t+1} = \arg\min_{\mathcal{U}_n} \left\{ \mathcal{L}_n(\mathcal{U}_n, V_n^{t+1}, Z_n), L(U) \mathcal{L}(U) = I_{r_n}, \text{ for } n \leq k, \right.$$  

$$\left. \mathcal{L}_n(\mathcal{U}_n, V_n^{t+1}, Z_n), R(U) \mathcal{R}(U)^T = I_{r_n}, \text{ for } n > k, \right.$$  

$$Z_n^{t+1} = Z_n^t - \gamma (V_n^{t+1} - U_n^{t+1}).$$

Once $V_n, U_n, Z_n$ are updated for all $n$, samples $X$ are computed using:

$$X^{t+1} = \arg\min_{X} \mathcal{L}(X^{t+1}, \{V_n^{t+1}\}, X_t, \{Z_n^{t+1}\}).$$

3.1.1. Solution for $\mathcal{V}_n$

For $n \leq k$, the solution for $V_n^{t+1}$ can be written explicitly as:

$$V_n^{t+1} = \mathcal{U}_n^T \mathcal{X} + \frac{\gamma}{2} \| \mathcal{V}_n - \mathcal{U}_n^T \mathcal{X} \|^2_F,$$

$$-Z_n^t \times_1 Z_n \times_2 \ldots \times_3 (V_n - U_n) + \frac{\gamma}{2} \| V_n - U_n \|^2_F.$$
\[
\begin{align*}
\gamma &= \arg\min_{\mathcal{V}_n} \|\mathbf{H}(\mathcal{V}_n)P - \mathbf{T}_n(\mathbf{\pi}_{k+1}(\mathcal{Y}))\|_F^2 \quad - \text{tr}\left(\mathbf{L}(\mathcal{Z}_n^t)^\top \mathbf{L}(\mathcal{V}_n - \mathbf{\mu}_n)\right) + \frac{\gamma}{2} \|\mathbf{L}(\mathcal{V}_n) - \mathbf{L}(\mathbf{\mu}_n)\|_F^2,
\end{align*}
\]
where \( H = \left[ \mathcal{I}_n \oplus V_{5,1}^{t+1} \right] \), \( P = \mathbf{R}(V_{5,1}^{t+1} \times \cdots \times V_{5,1}^{t+1}) \), \( \mathcal{V}_n \), \( \mathcal{Z}_n^t \), \( \mathbf{\mu}_n \), \( \mathbf{\mu}_n \), \( \mathbf{\pi}_{k+1}(\mathcal{Y}) \). The analytical solution is found by taking the derivative with respect to \( \mathbf{L}(\mathcal{V}_n) \) and setting it to zero:

\[
2\mathbf{H}^\top \left( H \mathbf{L}(\mathcal{V}_n^{t+1})P - G \right) P^\top - \mathbf{L}(\mathcal{Z}_n^t) + \gamma(\mathbf{L}(\mathcal{V}_n^{t+1}) - \gamma \mathbf{L}(\mathbf{\mu}_n)) = 0,
\]

\[
\mathbf{T}_3(\gamma \mathbf{\mu}_n - \mathcal{Z}_n^t) + 2\mathbf{T}_2(\mathbf{H}^\top \mathbf{G}^\top P^\top),
\]
where \( G = \mathbf{T}_n(\mathbf{\pi}_{k+1}(\mathcal{Y})) \). Note that the inverse in the solution will always exist given \( \gamma > 0 \) as the inverse of a sum of a Hermitian matrix and an identity matrix always exists.

When \( n < k \), following [11] the solution for \( \mathcal{V}_n \) can be written in the same manner but with different \( H, G \) and \( P \), where \( H = V_{5,1}^{t+1} \), \( P = V_{5,1}^{t+1} \), \( G = \mathbf{T}_n(\mathbf{\pi}_{k+1}(\mathcal{Y})) \). We show that these conditions hold for each optimization problem corresponding to mode \( n \). The gradient of \( f_{ij} \) with respect to \( \mathbf{V}_n \) is Lipschitz continuous with \( L \geq \|PP^\top \otimes H^\top H\|_2 \), which fulfills the conditions given in [20]. Thus, \( \mathcal{L}_n \) converges to a set of solutions \( \mathbf{V}_n^{k+1}, \mathbf{U}_n^{k+1}, \mathcal{Z}_n \) giving that \( \gamma \geq 2L + 1 \).

The solution for \( \mathcal{X} \) is found analytically. As the iterative solutions for each variable converge and the optimization function is nonnegative, i.e. bounded from below, the algorithm converges to a local minimum.

### 4. EXPERIMENTS

The proposed method is evaluated for clustering and compared to existing tensor clustering methods including k-means, MPS [15], TTNPE [11] and GLTD [13] for Weizmann Face Database and MNIST Dataset. Clustering quality is quantified by Normalized Mutual Information (NMI). Average accuracy with respect to both storage complexity and computation time over 20 experiments are reported for all methods.

In the following experiments, the storage complexity is quantified as the size of the tensor factors \( (\mathbf{U}_n, \mathbf{V}_n) \) and projections \( (\mathcal{X}_n, \mathcal{Y}_n) \). The varying levels of storage cost are obtained by varying \( r_n, s \) in the implementation of the tensor decomposition methods. Using varying levels of a truncation parameter \( \tau \in (0, 1] \), the singular values smaller than \( \tau \) times the largest singular value are discarded. The rest are used to determine ranks \( r_n \) for both TT-based and TD-based methods. For GRTT and TTNPE, the ranks are selected using TT-decomposition proposed in [21], while for GLTD truncated HOSVD was used. Computational complexity is quantified as the time it takes to learn the tensor factors. In order to compute the run time, for TT-based methods, each set of tensor factors is optimized until the change in the normalized difference between consecutive tensor factors is less than 0.01 or 50 iterations are completed.

The regularization parameter, \( \lambda \), for each experiment was selected using a validation set composed of a small batch of samples not included in the experiments. 5 random experiments were conducted and optimal \( \lambda \) was selected as the value that gave the best average NMI for a range of \( \lambda \) values from 0.001 to 1000 increasing in a logarithmic scale. The similarity graphs were constructed using

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**Algorithm 1** Graph Regularized Tensor Train-ADMM (GRTT-ADMM)

**Input:** Input tensors \( \mathcal{Y}_n \in \mathbb{R}^{t_1 \times t_2 \times \cdots \times t_N} \) where \( s \in \{1, \ldots, S\} \), initial tensor factors \( \{\mathcal{T}_i\}, n \in \{1, \ldots, N\}, k, \lambda, r_1, \ldots, r_N, \) \( \text{LoopIter}, \text{ConvThresh} \)

**Output:** \( \mathcal{U}_n, \mathcal{V}_n \in \{1, \ldots, N\}, \) and \( \mathcal{X}_n, \mathcal{Y}_n \)

1: \( \{\mathcal{T}_i\} \leftarrow \{\mathcal{U}_i\} \)
2: \( c \leftarrow 0 \)
3: while \( t < \text{LoopIter} \) or \( c > \text{ConvThresh} \) do
   4: for \( n = 1 : N \) do
      5: \( \text{Find} \mathcal{V}_n^{t+1} \) using (12).
      6: \( \text{Find} \mathcal{U}_n^{t+1} \) using SVD to solve (13).
      7: \( \text{Find} \mathcal{Z}_n^{t+1} \) using (6).
   8: end for
   9: \( c \leftarrow \frac{1}{N} \sum_{n=1}^{N} \|\mathcal{V}_n^{t+1} - \mathcal{V}_n^{t}\|_F^2 \)
10: \( t \leftarrow t + 1 \)
11: end while

Our objective function is nonconvex due to unitary constraints. In [20], it has been shown that this type of nonconvex optimization problems, i.e. convex optimization on a Stiefel manifold, converge under some conditions. We show that these conditions hold for each optimization problem corresponding to mode \( n \). The gradient of \( f_{ij} \) with respect to \( \mathbf{V}_n \) is Lipschitz continuous with \( L \geq \|PP^\top \otimes H^\top H\|_2 \), which fulfills the conditions given in [20]. Thus, \( \mathcal{L}_n \) converges to a set of solutions \( \mathbf{V}_n^{k+1}, \mathbf{U}_n^{k+1}, \mathcal{Z}_n \) giving that \( \gamma \geq 2L + 1 \).
k-nearest neighbor method with $k = \log(S)$ following [22].

4.1. MNIST

MNIST is a database of grayscale handwritten digit images where each image is of size $28 \times 28$. We transformed each of the images to a $4 \times 7 \times 4 \times 7$ tensor. Reshaping the inputs into higher order tensors is common practice and was employed in prior work [23] [21] [24] [14] [25]. In our experiments, we used a subset of 500 images with 50 images from each class. 50 samples with 5 samples from each class are used as validation set to determine $\lambda$.

**Fig. 1:** (a) Normalized Mutual Information vs. Storage Complexity of different methods for MNIST dataset. (b) Computation Time vs. Storage Complexity of different methods for MNIST dataset.

In Fig. 1a, we can see that at all storage complexity levels, our approach gives the best clustering result in terms of NMI. The dotted purple line represents the accuracy of k-means clustering on original tensor data. Even though the performance of TTNPE is the closest to our method, it is computationally inefficient. In Fig. 1b we can see that our approach is faster than GLTD and TTNPE at all storage complexities. MPS is the most efficient in terms of speed but it provides poor clustering quality.

4.2. COIL

The dataset consists of 7,200 RGB images of 100 objects of size $128 \times 128$. Each object has 72 images, where each image corresponds to a different pose angle ranging from 0 to 360 degrees with increments of 5 degrees [26]. We used a subset of 20 classes and 32 randomly selected, downsampled, grayscale samples from each class. Each image was converted to an $8 \times 8 \times 8 \times 8 \times 8$ tensor. 8 samples from each class are used as validation set.

From Fig. 2a we can see that the proposed method provides the best clustering results compared to all other methods. The results for GLTD seem to deteriorate with increasing ranks, which is a result of using orthonormal tensor factors. TTNPE gives results closest to the proposed method but it is computationally inefficient and gets very slow with increasing $r_{ns}$. From Fig. 2b we can see that MPS provides best results in terms of run time but the proposed method has a similar computational complexity while providing better clustering accuracy.

**Fig. 2:** (a) Normalized Mutual Information vs Storage Complexity of different methods for COIL dataset. (b) Computation Time vs Storage Complexity of different methods for COIL dataset.

5. CONCLUSIONS

In this paper, we proposed a unsupervised graph regularized tensor train decomposition for dimensionality reduction. To the best of our knowledge, this is the first tensor train based dimensionality reduction method that incorporates manifold information through graph regularization. The proposed method also utilizes a multi-branch structure to implement tensor train decomposition which increases the computational efficiency. An ADMM based algorithm is proposed to solve the resulting optimization problem. The proposed method was compared to GLTD, TTNPE and MPS for unsupervised learning in two different datasets.

The proposed method provided the best results in terms of clustering quality while being very efficient in terms of computational cost. The proposed method could also be employed in other dimensionality reduction applications such as denoising, data recovery, and compression. Future work will consider the selection of different design parameters such as the optimal tensor train structure, the construction of the similarity graph and the analysis of convergence rate. Future work will also consider extension of this framework to supervised learning applications.
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