Are Tensor Decomposition Solutions Unique?  
On the global convergence of HOSVD and ParaFac algorithms

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Abstract

For tensor decompositions such as HOSVD and ParaFac, the objective functions are nonconvex. This implies, theoretically, there exists a large number of local optima: starting from different starting point, the iteratively improved solution will converge to different local solutions. This non-uniqueness present a stability and reliability problem for image compression and retrieval. In this paper, we present the results of a comprehensive investigation of this problem. We found that although all tensor decomposition algorithms fail to reach a unique global solution on random data and severely scrambled data; surprisingly however, on all real life several data sets (even with substantial scramble and occlusions), HOSVD always produce the unique global solution in the parameter region suitable to practical applications, while ParaFac produce non-unique solutions. We provide an eigenvalue based rule for the assessing the solution uniqueness.

1. Introduction

Tensor based dimension reduction has recently been extensively studied for computer vision, pattern recognition, and machine learning applications. Typically, such approaches seek subspaces such that the information are retained while the discarded subspaces contains noises. Most tensor decomposition methods are unsupervised which enable researchers to apply them in any machine learning applications including unsupervised learning and semi-supervised learning.

Perhaps High Order Singular Value Decomposition (HOSVD) [?] [?] and Parallel Factors (ParaFac) are some of the most widely used tensor decompositions. Both of them could be viewed as extensions of SVD of a 2D matrix. HOSVD is used in computer vision by Vasilescu and Terzopoulos [?] while ParaFac is used in computer vision by Shashua and Levine [?]. More recently, Yang et al. [?] proposed a two dimensional PCA (2DPCA) Ye et al. [?] proposed a method called Generalized Low Rank Approximation of Matrices (GLRAM). Both GLRAM and 2DPCA can be viewed in the same framework in 2DSVD (two-dimensional singular value decomposition) [?], and solved by non-iterative algorithm [5] The error bounds of HOSVD have been derived [3] and the equivalence between tensor $K$-means clustering and HOSVD is also established [?].

Although tensor decompositions are now widely used, many of their properties so far have not been well characterized. For example, the tensor rank problem remains a research issue. Counter examples exist that argue against optimal low-dimension approximations of a tensor.

In this paper, we address the solution uniqueness issues. This problem arises because the tensor decomposition objective functions are non-convex with respect to all the variables and the constraints of the optimization are also non-convex. Standard algorithms to compute these decompositions are iterative improvement. The non-convexity of the optimization implies that the iterated solutions will converge to different solutions if they start from different initial points.

Note that this fundamental uniqueness issue differs from other representation redundancy issues, such as equivalence transformations (i.e. rational invariance) that change individual factors $(U, V, W)$ but leaves the reconstructed image untouched. These representation redundancy issues can be avoided if we compare different solutions at the level of reconstructed images, rather in the level of individual factors.

The main findings of our investigation are both surprising and comforting. On all real life datasets we tested (we tested 6 data sets and show results for 3 data set due to space limitation), the HOSVD solutions are unique (i.e., different initial starts always converge to an unique global solution); while the ParaFac solution are almost always not unique. Furthermore, even with substantial randomizations (block scramble, pixel scramble, occlusion) of these real datasets, HOSVD converge to unique solution too.

These new findings assure us that in most applications
using HOSVD, the solutions are unique — the results are repeatable and reliable.

We also found that whether a HOSVD solution is unique can be reasonably predicted by inspecting the eigenvalue distributions of the correlation matrices involved. Thus the eigenvalue distributions provide a clue about the solution uniqueness or global convergence. We are looking into a theoretical explanation of this rather robust uniqueness of HOSVD.

2. Tensor Decomposition

2.1. High Order SVD (HOSVD)

Consider 3D tensor: $X = \{X_{ijk}\}_{i,j,k=1}^{n_1,n_2,n_3}$. The objective of HOSVD is to select subspace $U,V,W$ and core tensor $S$ such that the $L_2$ reconstruction error is minimized,

$$\min_{U,V,W,S} J_1 = \|X - U \otimes_1 V \otimes_2 W \otimes_3 S\|^2$$

where $U \in \mathbb{R}^{n_1 \times m_1}$, $V \in \mathbb{R}^{n_2 \times m_2}$, $W \in \mathbb{R}^{n_3 \times m_3}$, $S \in \mathbb{R}^{m_1 \times m_2 \times m_3}$. Using explicit index,

$$J_1 = \sum_{ijk} \left(X_{ijk} - \sum_{pqr} U_{ip} V_{jq} W_{kr} S_{pqr}\right)^2.$$  \hspace{1cm} (2)

In HOSVD, $W, U, V$ are required to be orthogonal:

$$U^T U = I, \quad V^T V = I, \quad W^T W = I.$$  \hspace{1cm} (11)

With the orthonormality condition, setting $\partial J_1 / \partial S = 0$, we obtain $S = U^T \otimes_1 V^T \otimes_2 W^T \otimes_3 X$, and $J_1 = \|X\|^2 - \|S\|^2$. Thus HOSVD is equivalent to maximize

$$\max_{U,V,W} \|S\|^2 = \|U^T \otimes_1 V^T \otimes_2 W^T \otimes_3 X\|^2.$$  \hspace{1cm} (3)

$$= \text{Tr} U^T F U$$  \hspace{1cm} (4)

$$= \text{Tr} V^T G V$$  \hspace{1cm} (5)

$$= \text{Tr} W^T H W$$  \hspace{1cm} (6)

where

$$F_{ij'} = \sum_{jj'} X_{ijj'} (V V^T)_{jj'} (W W^T)_{ll'}$$  \hspace{1cm} (7)

$$G_{jj'} = \sum_{ii'} X_{ijj'} (U U^T)_{ii'} (W W^T)_{ll'}$$  \hspace{1cm} (8)

$$H_{ll'} = \sum_{ii'jj'} X_{ijj'} (U U^T)_{ii'} (V V^T)_{jj'}$$  \hspace{1cm} (9)

Standard HOSVD algorithm starts with initial guess of of $(U, V, W)$ and solve Eqs(3,4,5) alternatively using eigenvectors of the corresponding matrix. Since $F, G, H$ are semi-positive definite, $\|S\|^2$ are monotonically increase (non-decrease). Thus the algorithm converges to a local optimal solution.

HOSVD is a nonconvex optimization problem: The objective function of Eq.(2) w.r.t. $(U, V, W)$ is nonconvex and the orthonormality constraints of Eq.(2) are nonconvex as well. It is well-known that for nonconvex optimization problems, there are many local optimal solutions: starting from different initial guess of $(U, V, W)$, the converged solutions are different. Therefore theoretically, solutions of HOSVD are not unique.

2.2. ParaFac decomposition

ParaFac decomposition [4, 2] is the simplest and also most widely used decomposition model. It approximates the tensor as

$$X \approx \sum_{r=1}^{R} u^{(r)} \otimes v^{(r)} \otimes w^{(r)}, \quad \text{or} \quad X_{ijk} \approx \sum_{r=1}^{R} U_{ir} V_{jr} W_{kr}.$$  \hspace{1cm} (10)

where $R$ is the number of factors and $U = (u^{(1)}, \ldots , u^{(R)})$, $V = (v^{(1)}, \ldots , v^{(R)})$, $W = (w^{(1)}, \ldots , w^{(R)})$. ParaFac minimizes the objective

$$J_{\text{ParaFac}} = \sum_{i=1}^{n_1} \sum_{j=1}^{n_2} \sum_{k=1}^{n_3} \|X_{ijk} - \sum_{r=1}^{R} U_{ir} V_{jr} W_{kr}\|^2$$  \hspace{1cm} (11)

We enforce the implicit constraints that columns of $U = (u^{(1)}, \ldots , u^{(R)})$ are linearly independent; columns of $V = (v^{(1)}, \ldots , v^{(R)})$ are linearly independent; and columns of $W = (w^{(1)}, \ldots , w^{(R)})$ are linearly independent.

Clearly the ParaFac objective function is nonconvex in $(U, V, W)$. The linearly independent constraints are also nonconvex. Therefore, the ParaFac optimization is a nonconvex optimization.

Many different computational algorithms were developed for computing ParaFac. One type of algorithm uses a sequence of rank-1 approximations [10, 6, 2]. However, the solution of this heuristic approach differ from (local) optimal solutions.

The standard algorithm is to compute one factor at a time in an alternating fashion. The objective decrease monotonically in each step, and the iteration converges to a (local) optimal solution. However, due to the nonconvexity of ParaFac optimization, the converged solution depends heavily on the initial starting point. For this reason, the ParaFac is often not unique.

3. Unique Solution

In this paper, we investigate the problem of whether the solution of a tensor decomposition is unique. This is an
important problem, because if the solutions is not unique, then the results are not repeatable and the image retrieval is not reliable.

For a convex optimization problem, there is only one local optimal solution which is also the global optimal solution. For a non-convex optimization problem, there are many (often infinite) local optimal solutions: converged solutions of the HOSVD/ParaFac iterations depend on the initial starting point.

In this paper, we take the experimental approach. For a tensor decomposition we run many runs with dramatically different starting points. If the solutions of all these runs agree with each other (to computer machine precision), then we consider the decomposition has a unique solution.

In the following, we explain the (1) The dramatically different starting point for \((U, V, W)\). (2) Experiments on three different real life data sets. (3) Eigenvalue distributions which can predict the uniques of the HOSVD.

4. A natural starting point for \(W\): the T1 decomposition and the PCA solution

In this section, we describe a natural starting point for \(W\). Consider the T1 decomposition \([?]\)

\[
X_{ijk} \approx \sum_{k'=1}^{m_3} C_{ijk} W_{kk'}, \quad \text{or} \quad X_{ij} \approx \sum_{k'=1}^{m_3} C_{ij}^{(k')} W_{kk'}. \tag{12}
\]

\(C, W\) are obtained as the results of the optimization

\[
\min_{C, W} J_{t_1} = \sum_{k=1}^{m_3} ||X^{(k)} - \sum_{k'=1}^{m_3} C^{(r)} W_{kk'}||^2. \tag{13}
\]

This decomposition can be reformulated as the following:

\[
J_{t_1} = ||X||^2 - \text{Tr}(W^T \tilde{H} W), \tag{14}
\]

where

\[
\tilde{H}_{kk'} = \text{Tr}(X^{(k)} [X^{(k')}]^T) = \sum_{ij} X_{ijk} X_{ijk'}. \tag{15}
\]

\(C\) is given by \(C^{(r)} = \sum_{k=1}^{m_3} X^{(k)} W_{kk'}\).

This solution is also the PCA solution. The reason is the following. Let \(A = (a_1, \cdots, a_n)\) be a collection of 1D vectors. The corresponding covariance matrix is \(AA^T\) and Gram matrix is \(A^T A\). Eigenvectors of \(A^T A\) are the principal components. Coming back to the T1 decomposition, \(\tilde{H}\) is the Gram matrix if we consider each image \(X^{(k)}\) as a 1D vector. Solution for \(W\) are principal eigenvectors of \(\tilde{H}\), which are the principal components.

5. Initialization

For both HOSVD and ParaFac, we generate 7 different initializations:

- (R1) Use the PCA results \(W\) as explained in §4. Set \(V\) to identity matrix (fill zeros in the rest of the matrix to fit the size of \(n_2 \times n_3\)). This is our standard initialization.
- (R2) Generate 3 full-rank matrixes \(W\) and \(V\) with uniform random numbers of \(0, 1\).
- (R3) Randomly generate 3 rank deficient matrices \(W\) and \(V\) with proper size. For first initialization, we randomly pick a column of \(W\) and set the column to zero. The rest of columns are randomly generated as in (R2) and the same for \(V\). For second and third initializations, we randomly pick two or three columns of \(W\) and set them to zero, and so on. Typically, we use \(m_1 = m_2 = m_3 = 5 \approx 10\). Thus the rank-deficiency at \(m_3 = 5\) is strong.

We use the tensor toolbox \([1]\). The order of update in the alternating updating algorithm is the following: (1) Given \((V, W)\), solve for \(U\) (to solve Problem 4); (2) Given \((U, W)\), solve for \(V\) (Problem 5); (3) Given \((U, V)\), solve for \(W\) (Problem 6); Go back to (1) and so on.

6. Run statistics and validation

For each dataset with each parameter setting, we run 10 independent tests. For each test, we run HOSVD iterations to convergences (because of the difficulty of estimating convergence criterion, we run total of \(T=100\) iterations of alternating updating which is usually sufficient to converge).

For each independent test, we have 7 different solutions of \((U_i, V_i, W_i)\) where \(i = 1, 2, \cdots, 7\) for the solution starting from the \(i\)-th initialization. We use the following difference to verify whether the solutions are unique:

\[
d(t) = \frac{1}{6} \sum_{i=2}^{7} \left( ||U_i^t - U_i^t|| + ||V_i^t - V_i^t|| + ||W_i^t - W_i^t|| \right),
\]

where we introduce the HOSVD iteration index \(t\), and \(U_i^t, V_i^t, W_i^t\) are the solution in \(t\)-th iteration.

If an optimization problem has a unique solution, \(d(t)\) typically starts with nonzero value and gradually decrease to zero. Indeed, this occurs often in Figure 2. The sooner \(d(t)\) decreases to zero, the faster the algorithm converges. For example, in the 7th row of Figure 2, the \(m_1 = m_2 = m_3 = 5\) parameter setting, the algorithm converges faster than the \(m_1 = m_2 = m_3 = 10\) setting.

In our experiments, we do 10 different tests (each with different random starts). If in all 10 tests \(d(t)\) decreases to zero, we say the optimization has a unique solution (we say they are globally convergent).

If an optimization has no unique solution (i.e., it has many local optima), \(d(t)\) typically remains nonzero at all times, we say the solution of HOSVD is not unique. In Figure 1, we show the results of HOSVD and ParaFac on a random tensor. One can see that in each of the 10 tests, shown as 10 lines in the figure, none of them ever decrease to zero.
For ParaFac we use the difference of reconstructed tensor to evaluate the uniqueness of the solution:

\[ d^t(t) = \frac{1}{6} \sum_{i=2}^{7} \| \hat{X}_i^t - \tilde{X}_i^t \|, \]  

(16)

where \( \hat{X}_i^t \) is the reconstruction tensor in the \( t \)-th iteration with the \( i \)-th starting point. ParaFac algorithm converge slower than HOSVD algorithm. Thus we run 2000 iterations for each test.

7. Eigenvalue Distributions

In these figures, the eigenvalues of \( F, G, \) and \( H \) are calculated using Eqs.(7,8,9), but setting all \( UU^T, VV^T, W W^T \) as identity matrix. The matrices are centered in all indexes. The eigenvalues are sorted and normalized to form new images (see Figure 2).

Three types randomization are considered: block scramble, pixel scramble and occlusion. In block scramble, an image is divided into \( n = 2, 4, 8 \) blocks; blocks are scrambled to form new images (see Figure 2).

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In pixel sample, we randomly pick up \( \alpha = 40\%, 60\%, 80\% \) of the pixels in the image, and randomly scramble them to form a new image (see Figure 2).

We also experimented with occlusions with sizes upto half of the images. We found that occlusion consistently produce smaller randomization affects and HOSVD results converge to the unique solution. For this reason and the space limitation, we do not show the results here.

10. Main Results

From results shown in Figures 2, 3, and 4, we observe the following:

1. For all tested real-life data, ParaFac solutions are not unique, i.e., the converged solution depends on initial starts. This is consistent with the non-convex optimization as explained in §2.2.

2. For all tested real-life data, HOSVD solutions are unique, although theoretically, this is not guaranteed since the optimization of HOSVD is non-convex as explained in §2.1.

3. For even heavily rescrambled (randomized) real-life data, HOSVD solutions are also unique; This is surprising, given that the HOSVD optimization are non-convex.

4. For very severely rescrambled real-life data and pure randomly generated data, HOSVD solutions are not unique.

5. The HOSVD solution for a given dataset may be unique for some parameter setting but non-unique for some other parameter setting.

6. Whether the HOSVD solution for a given dataset will be unique can largely be predicted by inspecting the eigenvalue distribution of the matrices \( F, G, H \). See next section.

11. Eigenvalue-base uniqueness prediction

We found Empirically that the eigenvalue distribution help to predict whether the HOSVD solution on a dataset with a parameter setting is unique or not.

For example, in AT&T dataset HOSVD converges in all parameter settings except in \( 8 \times 8 \) block scramble with \( m_1 = m_2 = m_3 = 5 \). This is because the ignored 3 eigenmodes have very similar eigenvalues as the first five eigenvalues. It is ambiguous for HOSVD to select which of the 8 significant eigenmodes. Thus HOSVD fails to converge to a unique solution.

But when we increase \( m_1, m_2, m_3 \) to 10, all 8 significant eigenmodes can be selected and HOSVD converges.
to a unique solution. This also happens in the other two datasets (see the forth rows in top part of Figures 3 and 4).

For 80% pixel scramble in dataset WANG, when \( m_1 = m_2 = m_3 = 5, 10 \), HOSVD is ambiguous as to select eigenmodes because there are a large number of them with nearly identical eigenvalues around the cutoff. However, if we reduce the dimensions to \( m_1 = m_2 = 2, m_3 = 4 \) or \( m_1 = m_2 = m_3 = 3 \), this ambiguity is gone: HOSVD clearly selects the top 2 or 3 eigenmodes. converges (see the last row of the top panel in Figure 3). This same observation also applies to Caltech 101 dataset at 80% pixel scramble in 101 (see the last row of the top part of Figure 4).

For random tensor shown in Figure 1, the eigenvalues are nearly identical to each other. Thus for both parameter setting (\( m_1 = m_2 = m_3 = 5 \) and \( m_1 = m_2 = m_3 = 10 \)), HOSVD is ambiguous to selection eigenmodes and thus does not converge.

We have also investigated the solution uniqueness problem of the GLRAM tensor decomposition. The results are very close to HOSVD. We skip it due to space limitation.

12. Summary

In summary, for all real life datasets we tested, the HOSVD solution are unique (i.e., different initial starts always converge to an unique global solution); while the ParaFac solution are almost always not unique. These finding are new (to the best of our knowledge). They also surprising and comforting. We can be assured that in most applications using HOSVD, the solutions are unique — the results are reliable and repeatable. In the rare cases where the data are highly irregular or severely distored/randomized, our results indicate that we can predict whether HOSVD solution is unique by inspecting the eigenvalue distributions.

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Figure 2. AT&T dataset (400 images of size 112 × 92 each). Shown are eigenvalues of F, G, H, and solution uniqueness of HOSVD and ParaFac.
Figure 3. WANG dataset (300 images, $100 \times 100$ size for each). Shown are eigenvalues of $F$, $G$, $H$, and solution uniqueness of HOSVD and ParaFac.
Figure 4. Caltech 101 dataset (200 images of size 100 × 100 each). Shown are eigenvalues of $F, G, H$, and solution uniqueness of HOSVD and ParaFac.
