

**DIMENSIONALITY REDUCTION FOR HIGHER-ORDER
TENSORS: ALGORITHMS AND APPLICATIONS**

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Abstract: Higher-order tensors have applications in many areas such as biomedical engineering, image processing, and signal processing. For example, dimensionality reduction of a multi-way problem can be achieved by the best rank- (R_1, R_2, \dots, R_N) approximation of tensors. Contrary to the matrix case, the tensor best rank- (R_1, R_2, \dots, R_N) approximation cannot be computed in a straightforward way. In this paper, we present the higher-order orthogonal iterations and outline two new algorithms, based on the trust-region and conjugate gradient methods on manifolds. We touch on some of the applications.

AMS Subject Classification: 15A69, 15A18

Key Words: multilinear algebra, higher-order tensor, rank reduction, trust-region, conjugate gradients, Grassmann manifold

Received: August 17, 2007

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1. Motivation

Independent component analysis applications, such as electro-encephalography, magneto-encephalography, nuclear magnetic resonance, often involve high-dimensional data in which only a few sources have significant contributions. To reduce the dimensionality of the problem from the number of observation channels to the number of sources the best rank- (R_1, R_2, \dots, R_N) approximation of tensors can be used, see [6].

Parallel factor decomposition (PARAFAC) (see [9]) is a decomposition of higher-order tensors in rank-1 terms. This decomposition is widely used in chemometrics. It can also be used for epileptic seizure onset localisation (see [7]), since only one of its components is related to the seizure activity. However, computing PARAFAC is a difficult problem, especially if the dimensions of the tensor are large. Dimensionality reduction is useful in this case as well.

Another field in which the best rank- (R_1, R_2, \dots, R_N) approximation of tensors can be applied is image synthesis, analysis and recognition. A set of facial images can be represented as a higher-order tensor, where different modes correspond to different factors, such as face expression, position of the head relative to the camera, and illumination, see [10].

Finally, we mention that in many signal processing applications a signal is decomposed as a sum of exponentially damped sinusoids. Tensor-based algorithms for the estimation of the poles and the complex amplitudes, given only samples of the signal are proposed in [11]. They are based on the best rank- (R_1, R_2, \dots, R_N) approximation of a tensor.

This paper is organized as follows: Section 2 introduces the problem of the best rank- (R_1, R_2, R_3) approximation. For simplicity we only consider real-valued third-order tensors. The generalization to higher-order tensors is straightforward. One algorithm for solving the problem is the higher-order orthogonal iteration (HOOI) (see [5]) which is an alternating least-squares algorithm. It is summarized in Section 3. Two new algorithms, based on the trust-region and on the conjugate gradients methods on manifolds are outlined in Section 4 and Section 5 respectively. Another manifold-based algorithm was recently proposed in [8].

2. Problem Formulation

N th-order tensors are generalizations of vectors (order 1) and matrices (order 2). Their elements are referred to by N indices. The columns of a tensor are called mode-1 vectors, the rows are called mode-2 vectors. In general, the mode- n vectors ($n = 1, 2, \dots, N$) are the vectors, obtained by varying the n -th index, while keeping the other indices fixed. The maximal number of linearly independent mode- n vectors is called the mode- n rank. It is a generalization of the column and row rank of a matrix but different mode- n ranks are not necessarily equal to each other.

Our goal is the best rank- (R_1, R_2, R_3) approximation $\hat{\mathcal{A}} \in \mathbb{R}^{I_1 \times I_2 \times I_3}$ of a third-order tensor $\mathcal{A} \in \mathbb{R}^{I_1 \times I_2 \times I_3}$ as a tool for dimensionality reduction. $\hat{\mathcal{A}}$ needs to minimize the least-squares cost function $F : \mathbb{R}^{I_1 \times I_2 \times I_3} \rightarrow \mathbb{R}$,

$$F : \hat{\mathcal{A}} \mapsto \|\mathcal{A} - \hat{\mathcal{A}}\|^2 \tag{1}$$

under the constraints $\text{rank}_1(\hat{\mathcal{A}}) \leq R_1, \text{rank}_2(\hat{\mathcal{A}}) \leq R_2, \text{rank}_3(\hat{\mathcal{A}}) \leq R_3$, where $\text{rank}_n(\cdot)$ stands for the mode- n rank and $\|\cdot\|$ is the Frobenius norm. The truncated SVD gives the best low-rank approximation of a matrix. However, truncation of the higher-order equivalent of the SVD (HOSVD) (see [4]) usually results in a suboptimal tensor rank- (R_1, R_2, \dots, R_N) approximation, which can be refined by iterative algorithms.

In this paper, we consider maximizing \bar{g} ,

$$\bar{g} : (\mathbf{U}, \mathbf{V}, \mathbf{W}) \mapsto \|\mathcal{A} \bullet_1 \mathbf{U}^T \bullet_2 \mathbf{V}^T \bullet_3 \mathbf{W}^T\|^2, \tag{2}$$

over the orthonormal matrices $\mathbf{U}, \mathbf{V}, \mathbf{W}$. Here, $\mathcal{A} \bullet_n \mathbf{M}$, $n = 1, 2, 3$ is the product of a tensor \mathcal{A} and a matrix \mathbf{M} with respect to the n -th mode of the tensor, see [4]. This problem is equivalent to minimizing (1), see [5]. It is also possible to perform computations on a matrix level due to the following property of \bar{g}

$$\bar{g}(\mathbf{U}, \mathbf{V}, \mathbf{W}) = \|\mathcal{A} \bullet_1 \mathbf{U}^T \bullet_2 \mathbf{V}^T \bullet_3 \mathbf{W}^T\|^2 = \|\mathbf{U}^T (\mathbf{A}_{(1)}(\mathbf{V} \otimes \mathbf{W}))\|^2, \tag{3}$$

where $\mathbf{A}_{(1)}$ is a matrix representation of the tensor \mathcal{A} , obtained by putting the columns of \mathcal{A} one after the other in a specific order, see [4]. The symbol “ \otimes ” stands for the Kronecker product. Having estimated $\mathbf{U}, \mathbf{V}, \mathbf{W}$, the optimal tensor $\hat{\mathcal{A}}$ is computed (see [5]) by

$$\hat{\mathcal{A}} = \mathcal{B} \bullet_1 \mathbf{U} \bullet_2 \mathbf{V} \bullet_3 \mathbf{W}, \tag{4}$$

where $\mathcal{B} = \mathcal{A} \bullet_1 \mathbf{U}^T \bullet_2 \mathbf{V}^T \bullet_3 \mathbf{W}^T \in \mathbb{R}^{R_1 \times R_2 \times R_3}$.

3. Higher-Order Orthogonal Iteration

HOOI (see [5]) is an alternating least-squares algorithm for optimizing (2). At each step the estimate of one of the matrices $\mathbf{U}, \mathbf{V}, \mathbf{W}$ is optimized, while the other two stay fixed. In order to maximize with respect to the unknown orthonormal matrix \mathbf{U} , $\bar{g}(\mathbf{U}, \mathbf{V}, \mathbf{W})$ is thought of as a quadratic expression in the components of \mathbf{U} . From (3) it can be deduced that the columns of $\mathbf{U} \in \mathbb{R}^{I_1 \times R_1}$ should build an orthonormal basis for the left R_1 -dimensional dominant singular subspace of $\mathbf{A}_{(1)}(\mathbf{V} \otimes \mathbf{W})$, which can be obtained from the SVD of $\mathbf{A}_{(1)}(\mathbf{V} \otimes \mathbf{W})$. The optimization with respect to \mathbf{V} and \mathbf{W} is performed by analogy.

The **HOOI Algorithm** can be summarized as follows:

1. Obtain initial estimates $\mathbf{U}_0, \mathbf{V}_0, \mathbf{W}_0$, e.g., from HOSVD.
2. Iterate until convergence ($k = 0, 1, 2, \dots$):
 - Compute the columns of \mathbf{U}_{k+1} as orthonormal basis vectors of the R_1 -dimensional left dominant singular subspace of $\mathbf{A}_{(1)}(\mathbf{V}_k \otimes \mathbf{W}_k)$.
 - Compute the columns of \mathbf{V}_{k+1} as orthonormal basis vectors of the R_2 -dimensional left dominant singular subspace of $\mathbf{A}_{(2)}(\mathbf{W}_k \otimes \mathbf{U}_{k+1})$.
 - Compute the columns of \mathbf{W}_{k+1} as orthonormal basis vectors of the R_3 -dimensional left dominant singular subspace of $\mathbf{A}_{(3)}(\mathbf{U}_{k+1} \otimes \mathbf{V}_{k+1})$.
3. Compute $\hat{\mathcal{A}}$ using (4) with the converged \mathbf{U}, \mathbf{V} , and \mathbf{W} from Step 2.

4. Trust Region Based Algorithm

The algorithm that we present in this section is based on the trust-region (TR) method on manifolds, see [1]. Our motivation for using manifolds is the invariance property of the function \bar{g} from (2),

$$\bar{g}(\mathbf{U}, \mathbf{V}, \mathbf{W}) = \bar{g}(\mathbf{U}\mathbf{Q}^{(1)}, \mathbf{V}\mathbf{Q}^{(2)}, \mathbf{W}\mathbf{Q}^{(3)}), \quad (5)$$

where $\mathbf{Q}^{(i)}$, $i = 1, 2, 3$ are orthogonal matrices. (5) holds for any $\mathbf{U}, \mathbf{V}, \mathbf{W}$ (not necessarily orthonormal), so we can define a function $g : M \rightarrow \mathbb{R}$,

$$g([\mathbf{U}], [\mathbf{V}], [\mathbf{W}]) = \bar{g}(\mathbf{U}, \mathbf{V}, \mathbf{W}), \quad (6)$$

on the product manifold $M = Gr(R_1, I_1) \times Gr(R_2, I_2) \times Gr(R_3, I_3)$, where $Gr(R, I)$ denotes the Grassmann manifold of R -dimensional subspaces of \mathbb{R}^I and $[\mathbf{A}]$ stands for all matrices whose columns span the same subspace as the ones of \mathbf{A} . The elements of M are more complex but simplifications in the

formulas and better convergence results follow, which justify (6).

The trust-region method (see [3]) is an iterative algorithm for minimizing a cost function f . At each step a quadratic model m of f is minimized in a trust-region around the current iterate and thus an update η is computed. The quality of the model is evaluated and as a consequence, the new iterate is accepted or rejected and the trust-region radius is updated. Below, we summarize the TR-based algorithm for the cost function g from (6).

The **TR-based algorithm**:

1. Obtain initial iterate $\mathbf{X}_0 = \{\mathbf{U}_0, \mathbf{V}_0, \mathbf{W}_0\} \in M$.
2. Iterate until convergence ($k = 0, 1, 2, \dots$)

— Compute η_k as the solution of the trust-region subproblem

$$\min_{\eta \in T_{\mathbf{X}_k} M} m_{\mathbf{X}_k}(\eta), \text{ subject to } \langle \eta, \eta \rangle \leq \Delta_k^2, \text{ where}$$

$$m_{\mathbf{X}_k}(\eta) = g(\mathbf{X}_k) + \langle \text{grad } g(\mathbf{X}_k), \eta \rangle + \frac{1}{2} \langle \text{Hess } g(\mathbf{X}_k)[\eta], \eta \rangle.$$

— Compute the quotient $\rho_k = \frac{g(\mathbf{X}_k) - g(R_{\mathbf{X}_k}(\eta_k))}{m_{\mathbf{X}_k}(0_{\mathbf{X}_k}) - m_{\mathbf{X}_k}(\eta_k)}$.

— Set \mathbf{X}_{k+1} to be $R_{\mathbf{X}_k}(\eta_k)$ if ρ_k is big enough and \mathbf{X}_k otherwise.

— Set Δ_{k+1} to be $\frac{1}{4}\Delta_k$ if ρ_k is too small, $2\Delta_k$ if ρ_k is large, else Δ_k .

3. Compute \hat{A} using (4) with the converged $\mathbf{X} = \{\mathbf{U}, \mathbf{V}, \mathbf{W}\}$ from Step 2.

The function R is called *retraction*. It specifies how a new iterate in the direction of the tangent vector $\eta = (\mathbf{Z}_U, \mathbf{Z}_V, \mathbf{Z}_W)$ at a point $\mathbf{X} = (\mathbf{U}, \mathbf{V}, \mathbf{W})$ on the manifold is computed (for details see [1]). For the manifold M the following retraction can be used:

$$R_{(\mathbf{U}, \mathbf{V}, \mathbf{W})}(\mathbf{Z}_U, \mathbf{Z}_V, \mathbf{Z}_W) = (\text{qf}(\mathbf{U} + \mathbf{Z}_U), \text{qf}(\mathbf{V} + \mathbf{Z}_V), \text{qf}(\mathbf{W} + \mathbf{Z}_W)),$$

where qf denotes the Q factor of the thin QR decomposition. Finally, we mention that closed-form expressions for the gradient $\text{grad } g$, and the Hessian $\text{Hess } g$ can be obtained.

5. Conjugate Gradients Based Algorithm

In this section, we propose a conjugate gradient (CG) based algorithm for solving (1). Again we make use of the invariance property (5) and manifold idea (6). The CG method is an iterative method for minimizing a cost function. At each step a search direction is computed, which takes into account the previous

ones. More details about nonlinear CG on manifolds can be found in [2].

The **CG-based algorithm** can be summarized as follows:

1. Obtain initial iterate $\mathbf{X}_0 = \{\mathbf{U}_0, \mathbf{V}_0, \mathbf{W}_0\} \in M$.
2. Set $\eta_0 = -\text{grad } g(\mathbf{X}_0)$.
3. Iterate until convergence ($k = 0, 1, 2, \dots$):
 - Compute α_k ; e.g., use Armijo stepsize.
 - Set $\mathbf{X}_{k+1} = R_{\mathbf{X}_k}(\alpha_k \eta_k)$.
 - Compute β_{k+1} , e.g., via the Fletcher-Reeves formula

$$\beta_{k+1} = \frac{\langle \text{grad } g(\mathbf{X}_{k+1}), \text{grad } g(\mathbf{X}_{k+1}) \rangle}{\langle \text{grad } g(\mathbf{X}_k), \text{grad } g(\mathbf{X}_k) \rangle}.$$
 - Set $\eta_{k+1} = -\text{grad } g(\mathbf{X}_{k+1}) + \beta_{k+1} \mathcal{T}_{\alpha_k \eta_k}(\eta_k)$.
4. Compute $\hat{\mathcal{A}}$ using (4) with the converged $\mathbf{X} = \{\mathbf{U}, \mathbf{V}, \mathbf{W}\}$ from Step 3.

To perform a CG algorithm on a manifold we need to work simultaneously with tangent vectors at two different points on the manifold. For this purpose we define a function, called *vector transport*, see [2]. For our problem, it can be the following function

$$\mathcal{T}_{\eta_{\mathbf{x}}} \xi_{\mathbf{x}} = P_{\mathbf{x} + \bar{\eta}_{\mathbf{x}}}^h \bar{\xi}_{\mathbf{x}},$$

where $\eta_{\mathbf{x}}$ and $\xi_{\mathbf{x}}$ are two tangent vectors at point $[\mathbf{X}]$, $\bar{\xi}$ is a matrix representation of ξ , called horizontal lift, and $P_{\mathbf{y}}^h$ is the projection onto the orthogonal complement of the column space of \mathbf{Y} .

Acknowledgements

The research reported in this paper is supported by:

- (i) FWO-G.0321.06 (Tensors/Spectral Analysis),
- (ii) IUAP P6/04 (DYSCO), 2007-2011,
- (iii) Impulsfinanciering Campus Kortrijk (2007-2012)(CIF1),
- (iv) Research Council KUL: OE/06/25, OE/07/17, GOA-AMBioRICS, CoE EF/05/006.

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