APPROXIMATE RANK-DETECTING FACTORIZATION OF LOW-RANK TENSORS

Franz J. Király

Machine Learning Group, Computer Science

Berlin Institute of Technology (TU Berlin)

Franklinstr. 28/29, 10587 Berlin, Germany

and Discrete Geometry Group, Institute of Mathematics, FU Berlin

and Mathematisches Forschungsinstitut Oberwolfach

Andreas Ziehe

Machine Learning Group, Computer Science

Berlin Institute of Technology (TU Berlin)

Franklinstr. 28/29, 10587 Berlin, Germany

ABSTRACT

We present an algorithm, AROFAC2, which detects the (CP-)rank of a degree 3 tensor and calculates its factorization into rank-one components. We provide generative conditions for the algorithm to work and demonstrate on both synthetic and real world data that AROFAC2 is a potentially outperforming alternative to the gold standard PARAFAC over which it has the advantages that it can intrinsically detect the true rank, avoids spurious components, and is stable with respect to outliers and non-Gaussian noise.

Index Terms— Tensor Decomposition, Tensor Factorization, Approximate Algebra, Simultaneous Diagonalization

1. INTRODUCTION

Polyadic decomposition of tensors into their canonical components (= canonic polyadic resp. CP-decomposition) and determining the number of those (= the rank) is a multidimensional generalization of the Singular Value Decomposition and the matrix rank, and a reoccurring task in all practical sciences, appearing many times under different names; first discovered by Hitchcock [1] and then re-discovered under names such as PARAFAC [2] or CANDECOMP [3], it has been applied in many fields such as chemometrics, psychometrics, and signal processing [4, 5, 6]. An extensive survey of many applications can be found in [7, 8].

Considerable effort has been devoted to develop theory and methodology for the CP-decomposition, however many fundamental issues are still unresolved. The mathematical theory concerning CP-decompositions of tensors which are not matrices is only partly understood; also, while there exist several methods to calculate the CP-decomposition of a tensor [9, 10], they are extrinsical in the sense that a structure-agnostic loss function is optimized and also highly sensitive to outliers or non-Gaussian noise - problems which have been heuristically attempted to cope with (e.g. [11]). Moreover, determining the rank of a noisy tensor remains a problematic task despite the existence of heuristics [12].

In this paper, we present AROFAC2, a method for calculating the CP-decomposition of a low-rank degree 3 tensor and its rank, which is based on theoretical considerations and intrinsical calculations making use of the algebraic structure of degree 3 tensors, part of which have already surfaced in [13]. Specifically, we show how the algebraic structure can be used to obtain components one-by-one by alternating projections - a technique which draws inspiration from [14] - and how to reduce determination of rank to a clustering problem. Due to its structure-awareness, our algorithm only finds the numerically stable components while avoiding spurious ones, and determines the correct rank; it is also less sensitive to outliers or noise. We demonstrate its superiority to existing approaches on synthetic data and a chemometrics data set.

2. TENSOR FACTORIZATION AND SIMULTANEOUS SVD

We briefly review the basic definitions of rank-one tensor decomposition, and introduce some notation.

Notations 2.1. *The set of $(n_1 \times n_2 \times n_3)$-tensors of degree 3 is denoted by*

$$\mathbb{C}^{n_1 \times n_2 \times n_3} = \left\{ (a_{ijk})_{\substack{1 \leq i \leq n_1 \\ 1 \leq j \leq n_2 \\ 1 \leq k \leq n_3}} \right\}.$$

For $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$, the matrices

$$A_1, \dots, A_{n_3} \quad \text{with } A_k = (a_{ijk})_{\substack{1 \leq i \leq n_1 \\ 1 \leq j \leq n_2}}$$

are called the 3-slices of A.

Definition 2.2. *Let $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$. Then, a decomposition*

$$A = \sum_{i=1}^{r} u_i \otimes v_i \otimes w_i \quad \text{with } u_i \in \mathbb{C}^{n_1}, v_i \in \mathbb{C}^{n_2}, w_i \in \mathbb{C}^{n_3},$$

is called a rank r canonic polyadic decomposition (or CP-decomposition) of A. The u_i, v_i, w_i are called (rank-one-)components of A. The u_i are called mode-1-, the v_i are

called mode-2-, and the w_i mode-3-components. The tensors $u_i \otimes v_i \otimes w_i$ are called (rank-one-)factors.

The (CP-)rank of A, denoted by $\mathrm{rk}(A)$, is the smallest r such that A has a rank r CP-decomposition.

This paper proposes an algorithmic solution for the following problem:

Problem 2.3. *Let $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$. Determine $r = \mathrm{rk}(A)$ and a rank r CP-decomposition of A.*

and for its approximate version, i.e., the case where A is noisy but of low tensor rank, and one wants to find a CP-decomposition of the noiseless A.

Related to that is the problem of finding a simultaneous singular value decomposition (SVD):

Problem 2.4. *Let $A_1, \ldots, A_{n_3} \in \mathbb{C}^{n_1 \times n_2}$. Determine a rank r, matrices $U \in \mathbb{C}^{n_1 \times r}, V \in \mathbb{C}^{n_2 \times r}$ and diagonal matrices $W_1, \ldots, W_{n_3} \in \mathbb{C}^{r \times r}$ such that*

$$A_k = U \cdot W_k \cdot V^\top \quad \text{for all } 1 \leq k \leq n_3.$$

In fact, Problems 2.3 and 2.4 are equivalent. We briefly prove that and add one additional characterization which will be important in the application:

Proposition 2.5. *Let $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$, let $A_1, \ldots, A_{n_3} \in \mathbb{C}^{n_1 \times n_2}$ be the 3-slices of A. Then, the following are equivalent:*
(i) A is a tensor of rank r in the sense of Definition 2.2.
(ii) The A_i have a simultaneous SVD of rank r in the sense of Problem 2.4.
(iii) There are rank one matrices $M_1, \ldots, M_r \in \mathbb{C}^{n_1 \times n_2}$ and coefficients $\lambda_{ij} \in \mathbb{C}, 1 \leq i \leq n_3, 1 \leq j \leq r$, such that

$$A_i = \sum_{j=1}^{r} \lambda_{ij} M_j \quad \text{for all } 1 \leq i \leq n_3.$$

Proof. (i)⇔(ii): There is only a notational difference which results from writing the columns of U as u_i, the columns of V as v_i, and, for i fixed and k running, the vectors formed by the i-th diagonal entries of the W_k as w_i, and the A_k as the 3-slices of A.
(i)⇔(iii): Again, the difference is only notational. Write $M_i = u_i \otimes v_i$ and λ_{ij} the i-th component of w_j. $\qquad\square$

3. UNIQUENESS OF CP-DECOMPOSITION AND LINEAR FACTORING

By the definitions above, it is not a-priori clear whether the CP-decomposition, including terminology such as component or factor, is well-defined, in particular whether it is unique. The method we present in this paper exploits certain properties of tensors with low rank. The main assumption on the tensor A to factor is the following:

Assumption 3.1. $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}, \mathrm{rk}(A) \leq \min(n_1, n_2, n_3)$.

It is probably known or folklore that in this case the CP-decomposition is unique, nevertheless we were not able to retrieve an exact reference. Thus, we provide a proof instead (for the notion of genericity, consult the appendix of [15]):

Theorem 3.2. *Let $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$ be generic with rank $\mathrm{rk}(A) = r \leq \min(n_1, n_2, n_3)$, let*

$$A = \sum_{i=1}^{r} u_i \otimes v_i \otimes w_i \quad \text{with } u_i \in \mathbb{C}^{n_1}, v_i \in \mathbb{C}^{n_2}, w_i \in \mathbb{C}^{n_3}$$

be a CP-decomposition of A. Then any CP-decomposition of A can be obtained by replacing the u_i, v_i, w_i by $\lambda_i u_i, \nu_i v_i, \lambda_i^{-1} \nu_i^{-1} w_i$, where $\lambda_i, \nu_i \in \mathbb{C}^\times$ for $1 \leq i \leq r$.

Proof. Keep the notation from Proposition 2.5, including A_i and M_j. Due to the observation in the proof of Proposition 2.5 that (i) and (iii) differ only in notation, the statement of this theorem is equivalent to proving that there is only one unique way to present the A_i as

$$A_i = \sum_{j=1}^{r} \lambda_{ij} M_j \quad \text{for all } 1 \leq i \leq n_3.$$

with rank one matrices M_j and numbers λ_{ij}, up to renumbering and the obvious rescaling by replacing M_j with $\mu_j M_j$ and λ_{ij} with $\mu_j^{-1} M_j$. Now since A is generic, the M_j are generic rank-one matrices, and the λ_{ij} are generic numbers. Thus, interpreting the A_i as rows of a $(n_3 \times n_1 n_2)$-matrix $\tilde{A}$, the M_j as rows of a $(r \times n_1 n_2)$-matrix M, and the λ_{ij} as elements of a $(n_3 \times r)$-matrix Λ. The presentation above can be reformulated as $\tilde{A} = \Lambda M$. The assumption $n_3 \leq r$ and Proposition 2.5 (iii) thus imply that the M_j lie in the span of the A_i. Now since the λ_{ij} are generic, Λ is a completely generic matrix. Thus, a different presentation of $\tilde{A}$ would correspond to the existence of an invertible $(r \times r)$ matrix P such that $\tilde{A} = \Lambda P^{-1} M'$ with a matrix M' whose rows correspond to rank-one-matrices, i.e., $M' = PM$. But a linear combination

$$M_i' = \sum_{i=1}^{r} p_{ij} M_j$$

of the $(n_1 \times n_2)$ matrices M_j has rank one if and only if exactly one of the p_{ij} (with i fixed) is non-zero, since $r \leq \min(n_1, n_2)$. Since P is of full rank, this implies that P is the product of a $(r \times r)$ permutation matrix with a full rank diagonal $(r \times r)$ matrix. But this is, as stated above, equivalent to the statement to prove. $\qquad\square$

Thus, under our assumptions components are unique up to scaling and numbering, and factors are unique up to numbering.

Proposition 2.5, together with the uniqueness guarantee in Theorem 3.2, gives the following statement:

Proposition 3.3. *Let $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$ be generic with rank* $\mathrm{rk}(A) = r \leq n_3$, *let* $A_1, \ldots, A_{n_3} \in \mathbb{C}^{n_1 \times n_2}$ *be the 3-slices of A. Then, up to scaling, there are r unique vectors* $\lambda^{(1)}, \ldots, \lambda^{(r)} \in \mathbb{C}^{n_3}$ *such that*

$$M(\lambda^{(k)}) = \sum_{i=1}^{n_3} \lambda_i^{(k)} A_i$$

has rank one. Moreover, for each k, let $M(\lambda^{(k)}) = u_k \otimes v_k$ be the (rank-one-)SVD. Then, the u_k and v_k are mode-1- and mode-2-components of A, belonging to the same factor.

4. THE AROFAC2 ALGORITHM

We propose an algorithm which computes rank and CP-decomposition of a degree 3 tensor A. It uses the routine `FindRankOne` which finds mode-1- and -2-components which we will present first as Algorithm 1. In step 1, the tensor is first decomposed into 3-slices A_i. In step 2, an approximate representation V for their span is calculated. This can be a PCA of the A_i, i.e., principal values or components, or a numerical span of lower dimension (if the true rank of A is known, the dimension should equal the rank). In step 3 a matrix $M \in V$ is randomized. This can be a random matrix in an exact span, or a matrix which is, e.g., sampled from a Gaussian with covariance matrix follows the estimated sample distribution of the A_i. Then steps 5 and 6, are repeated until convergence of M is attained. Step 5 takes (a possibly non-square) M to its third power, magnifying its largest singular value and diminishing the others. Step 6 projects M onto V and normalizes the result. Projection can be achieved by exact projection, or re-scaling, e.g., according to the principal values of the A_i. After convergence is reached, M will be approximately of rank one, and its first singular vectors, which are obtained in step 8, will be estimates for a mode-1- and a mode-2-component of A.

Algorithm 1 `FindRankOne`(A) *Input:* $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$
Output: One random mode-1-component $u \in \mathbb{C}^{n_1}$ and one random mode-2-component $v \in \mathbb{C}^{n_2}$ of A in the same factor.

1: Let $A_1, \ldots, A_{n_3}$ be the 3-slices of A.
2: Calculate an approximate representation V of $\mathrm{span}\langle A_1, \ldots, A_{n_3} \rangle$.
3: Randomize $M \in V$.
4: **repeat**
5: $\quad M \leftarrow M \cdot M^\top \cdot M$
6: $\quad M \leftarrow \mathcal{P}_V(M)$
7: **until** M has converged
8: Calculate approximate rank-one SVD of $M = u \cdot v^\top$
9: Return u, v

Algorithm 2 uses Algorithm 1 to obtain a full CP-decomposition and an estimate for the rank of A. In step 1, several candidate estimates for components of all modes are

obtained. Mode-3-components can be obtained by switching coordinates in A (e.g., switch the first with the third). If the mode-3-components are not relevant for the problem at hand, e.g., in the setting of simultaneous SVD as in Problem 2.4, this can be omitted. In steps 2 and step 3, a clustering algorithm is applied to estimate the number of cluster centers and cluster the candidate components. This can be done by different methods, or one single algorithm. Our implementation uses the mean shift algorithm which also estimates the number of cluster centers [16]. Since Algorithm 1 links pairs of components, this information can then be applied in step 4 to the estimated cluster centers in order to link pairs to full triples (which is unnecessary if only the first two modes are considered), e.g., by majority vote or vote weighted by closeness of a pair to the cluster center. The corresponding decomposition is then presented as the estimated solution in step 5.

Algorithm 2 `AROFAC2`(A) *Input:* $A \in \mathbb{C}^{n_1 \times n_2 \times n_3}$
Output: Rank and approximate CP-decomposition of A.

1: Repeat `FindRankOne`(A) to find sets $\mathcal{S}_1, \mathcal{S}_2, \mathcal{S}_3$ of potential mode-1-,-2-, and -3-components of A.
2: Use clustering algorithm to determine number r of clusters for $\mathcal{S}_1, \mathcal{S}_2$, and $\mathcal{S}_3$
3: Cluster $\mathcal{S}_1, \mathcal{S}_2$, and $\mathcal{S}_3$ to obtain cluster centers $u_1, \ldots, u_r$ of $\mathcal{S}_1$, centers $v_1, \ldots, v_r$ of $\mathcal{S}_2$ and $w_1, \ldots, w_r$ of $\mathcal{S}_3$.
4: Use the information from `FindRankOne`(A) to renumber the u_i, v_j, w_k such that for each ℓ, the components u_ℓ, v_ℓ, w_ℓ belong to the same factor.
5: Return r as the rank of A and $A = \sum_{i=1}^r u_i \otimes v_i \otimes w_i$ as its CP-decomposition.

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5. EXPERIMENTS

First, we demonstrate our algorithm on simulated toy data. The input tensor consists of 3-slices $A_k = \sum_{i=1}^r \lambda_{ik} u_i v_i^\top$ compare Proposition 2.5. Each slice is generated as follows: Exact singular vectors $u_i \in \mathbb{R}^{n_1}$, $v_i \in \mathbb{R}^{n_2}$, $1 \leq i \leq r$ are sampled independently and uniformly from the n_1-sphere and n_2-sphere, respectively. The λ_{ik} are sampled independently and uniformly from the standard normal distribution. Then, to each matrix $A_k, 1 \leq k \leq n_3$, noise is added in the form of a $(n_1 \times n_2)$ matrix whose entries are independently sampled from a normal distribution with mean 0 and covariance $\varepsilon \in \mathbb{R}^+$. Figure 1(a) shows the accuracy of the estimated U and V for $n_1 = 50, n_2 = 60, n_3 = 70, r = 10, \varepsilon = 0.1$ for PARAFAC (top row) vs AROFAC2 (bottom row). The estimation quality is essentially the same, however for AROFAC2 the correct rank $r = 10$ has been detected automatically.

In a second numerical evaluation, we analyze the noise robustness of the AROFAC2 algorithm. The data is generated
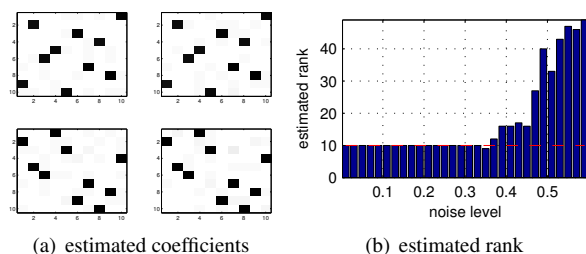
(a) estimated coefficients   (b) estimated rank

Fig. 1. (a) Absolute values of the correlation coefficients between the true and estimated components for PARAFAC (top row) vs AROFAC2 (bottom row). The correct solution has the same support as a permutation matrix. (b) Estimated rank for increasing noise levels ε. True rank is $r = 10$.

as before, but the noise level ε is increased from $\varepsilon = 0.01$ to $\varepsilon = 0.6$. In Figure 1(b) we see, that the correct rank $r = 10$ has been found for $\varepsilon \leq 0.35$ and is mainly overestimated for larger noise levels.

Finally we apply our algorithm to a publicly available data set from chemometrics. The **Dorrit fluorescence data** [17, 18] contains 27 synthetic samples of different mixtures of four analytes (hydroquinone, tryptophan, phenylalanine and DOPA) that were measured in a Perkin-Elmer LS50 B fluorescence spectrometer. The measurements of emission spectra at multiple excitation wavelengths give rise to an excitation-emission matrix (EEM) for each sample and thus form a degree 3 tensor which is known to obey the trilinear model where the rank is determined by the number of fluorophores [17, 18, 11]. As described in [19] this data set is highly suited to assess the performance of different methods due to its realistic noise from the physical environment and the availability of a priori knowledge of the underlying components. Figure 2 shows the estimated emission and excitation spectra for PARAFAC with 4 and 5 components and AROFAC2 with auto-detected 5 components. We note that the results of AROFAC2 are in excellent agreement with the known spectra (cf. Figs. 2 and 3 in [11]) while the components found by PARAFAC lack accuracy. In addition we observe that the AROFAC2 loadings better fulfill the non-negativity constraints even though they were not enforced explicitly. Furthermore, the peak of the fifth component around 315 nm in both excitation and emission spectra which can be attributed to Rayleigh scatter in all samples [20, 11] is sharper and thus in better agreement with its expected shape when identified by AROFAC2.

6. CONCLUSION

With AROFAC2, we have presented an algorithm which can determine the CP-decomposition and the rank of a potentially noisy degree three tensor. We argue that due to how the
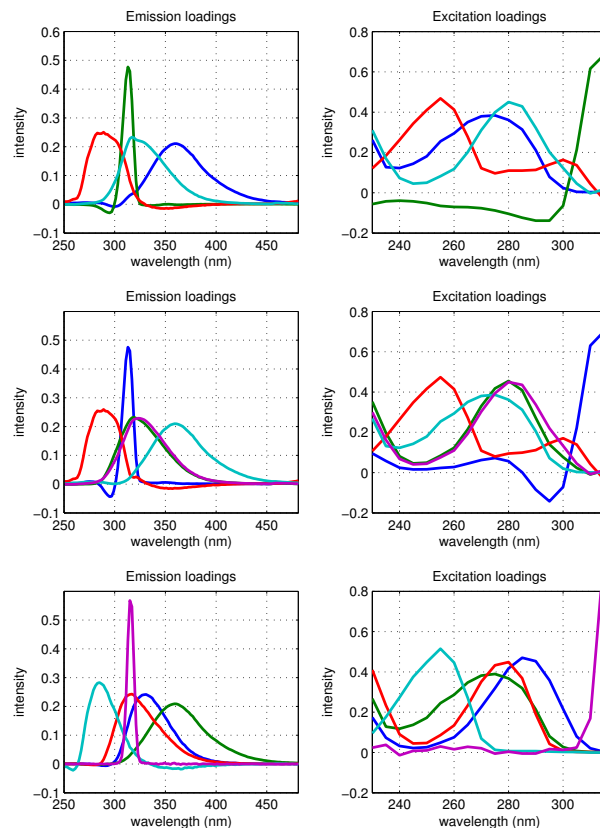

Fig. 2. Emission (left) and excitation (right) spectra for the Dorrit data using PARAFAC with $r = 4$ (top row) PARAFAC with $r = 5$ (middle row) and AROFAC2 with $r = 5$ automatically detected (bottom row).

algorithm is constructed, spurious and unstable components in the decomposition are not found; since the convergence criterion intrinsically enforces stability and thus informativeness of any found component. Our simulations demonstrate that AROFAC2 is competitive to the state-of-the-art method PARAFAC, but without the need to provide the true rank in advance. Also, AROFAC2 outperforms PARAFAC on the Dorrit data set which shows that AROFAC2 is a method which is more stable to outliers and the influence of non-Gaussian noise.

AROFAC2 uses the intrinsic algebraic structure of a low-rank degree tensor in the calculations, as opposed to most standard methods such as PARAFAC which assume a model and try to fit it, agnostic of its inner structure. We thus argue that algorithms exploiting this structure are to prefer whenever available, and the proper starting point for any method approaching any problem with algebraic features. We emphasize the potential benefit from applying structural insights to construct structure-aware methods.

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