# APPROXIMATE RANK-DETECTING FACTORIZATION OF LOW-RANK TENSORS 

Franz J. Király<br>Machine Learning Group, Computer Science<br>Berlin Institute of Technology (TU Berlin)<br>Franklinstr. 28/29, 10587 Berlin, Germany<br>and Discrete Geometry Group, Institute of Mathematics, FU Berlin<br>and Mathematisches Forschungsinstitut Oberwolfach

Andreas Ziehe<br>Machine Learning Group, Computer Science<br>Berlin Institute of Technology (TU Berlin)<br>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

[^0]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 structureagnostic 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 $\left(n_{1} \times n_{2} \times n_{3}\right)$-tensors of degree 3 is denoted by $\mathbb{C}^{n_{1} \times n_{2} \times n_{3}}$. For $A \in \mathbb{C}^{n_{1} \times n_{2} \times n_{3}}$, the matrices

$$
A_{1}, \ldots, A_{n_{3}} \quad \text { with } A_{k}=\left(a_{i j k}\right)_{\substack{1 \leq i \leq n_{1} \\ 1 \leq j \leq n_{2}}}
$$

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
$A=\sum_{i=1}^{r} u_{i} \otimes v_{i} \otimes w_{i} \quad$ 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 CPdecomposition) 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 ( $C P$-)rank of $A$, denoted by $\operatorname{rk}(A)$, is the smallest $r$ such that $A$ has a rank $r C P$-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 $r=\operatorname{rk}(A)$ 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 CPdecomposition 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 $A_{k}=U \cdot W_{k} \cdot V^{\top}$ 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 $\lambda_{i j} \in \mathbb{C}, 1 \leq i \leq n_{3}, 1 \leq j \leq r$, such that

$$
A_{i}=\sum_{j=1}^{r} \lambda_{i j} M_{j} \quad \text { for all } 1 \leq i \leq n_{3}
$$

Proof. (i) $\Leftrightarrow$ (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) $\Leftrightarrow$ (iii): Again, the difference is only notational. Write $M_{i}=u_{i} \otimes v_{i}$ and $\lambda_{i j}$ the $i$-th component of $w_{j}$.

## 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. $A \in \mathbb{C}^{n_{1} \times n_{2} \times n_{3}}, \operatorname{rk}(A) \leq \min \left(n_{1}, n_{2}, n_{3}\right)$.
It is probably known or folklore that in this case the CPdecomposition 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 $\operatorname{rk}(A)=r \leq \min \left(n_{1}, n_{2}, n_{3}\right)$, let
$A=\sum_{i=1}^{r} u_{i} \otimes v_{i} \otimes w_{i} \quad$ 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 $C P$-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

$$
A_{i}=\sum_{j=1}^{r} \lambda_{i j} M_{j} \quad \text { for all } 1 \leq i \leq n_{3}
$$

with rank one matrices $M_{j}$ and numbers $\lambda_{i j}$, up to renumbering and the obvious rescaling by replacing $M_{j}$ with $\mu_{j} M_{j}$ and $\lambda_{i j}$ with $\mu_{j}^{-1} M_{j}$. Now since $A$ is generic, the $M_{j}$ are generic rank-one matrices, and the $\lambda_{i j}$ are generic numbers. Thus, interpreting the $A_{i}$ as rows of a $\left(n_{3} \times n_{1} n_{2}\right)$-matrix $\tilde{A}$, the $M_{j}$ as rows of a $\left(r \times n_{1} n_{2}\right)$-matrix $M$, and the $\lambda_{i j}$ as elements of a $\left(n_{3} \times r\right)$-matrix $\Lambda$. 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 $\lambda_{i j}$ are generic, $\Lambda$ 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 $\tilde{A}=\Lambda P^{-1} M^{\prime}$ with a matrix $M^{\prime}$ whose rows correspond to rank-one-matrices, i.e., $M^{\prime}=P M$. But a linear combination

$$
M_{i}^{\prime}=\sum_{i=1}^{r} p_{i j} M_{j}
$$

of the $\left(n_{1} \times n_{2}\right)$ matrices $M_{j}$ has rank one if and only if exactly one of the $p_{i j}$ (with $i$ fixed) is non-zero, since $r \leq$ $\min \left(n_{1}, n_{2}\right)$. 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.

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 $\operatorname{rk}(A)=r \leq n_{3}$, 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

$$
M\left(\lambda^{(k)}\right)=\sum_{i=1}^{n_{3}} \lambda_{i}^{(k)} A_{i}
$$

has rank one. Moreover, for each $k$, let $M\left(\lambda^{(k)}\right)=u_{k} \otimes v_{k}$ 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 CPdecomposition 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-1and 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.
    Let \(A_{1}, \ldots, A_{n_{3}}\) be the 3 -slices of \(A\).
        Calculate an approximate representation \(V\) of
    \(\operatorname{span}\left\langle A_{1}, \ldots, A_{n_{3}}\right\rangle\).
    Randomize \(M \in V\).
    repeat
        \(M \leftarrow M \cdot M^{\top} \cdot M\)
        \(M \leftarrow \mathcal{P}_{V}(M)\)
    until \(M\) has converged
    Calculate approximate rank-one SVD of \(M=u \cdot v^{\top}\)
    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 .

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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 po-
    tential mode-1-,-2-, and -3-components of \(A\).
    2: Use clustering algorithm to determine number \(r\) of clus-
    ters 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 renum-
    ber the \(u_{i}, v_{j}, w_{k}\) such that for each \(\ell\), the components
    \(u_{\ell}, v_{\ell}, w_{\ell}\) 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.
```


## 5. EXPERIMENTS

First, we demonstrate our algorithm on simulated toy data. The input tensor consists of 3 -slices $A_{k}=\sum_{i=1}^{r} \lambda_{i k} u_{i} v_{i}^{\top}$ 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 $\lambda_{i k}$ 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


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 $\varepsilon$. True rank is $r=10$.
as before, but the noise level $\varepsilon$ 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 nonnegativity 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 nonGaussian noise.

AROFAC2 uses the intrinsic algebraic structure of a lowrank 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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