Abstract—The canonical polyadic decomposition (CPD) is a fundamental tensor decomposition which expresses a tensor as a sum of rank one tensors. In stark contrast to the matrix case, with light assumptions, the CPD of a low rank tensor is (essentially) unique. The essential uniqueness of CPD makes this decomposition a powerful tool in many applications as it allows for extraction of component information from a signal of interest.

One popular algorithm for algebraic computation of a CPD is the generalized eigenvalue decomposition (GEVD) which selects a matrix subpencil of a tensor, then computes the generalized eigenvectors of the pencil. In this article, we present a simplification of GEVD which improves the accuracy of the algorithm. Surprisingly, the generalized eigenvector computation in GEVD is in fact unnecessary and can be replaced by a QZ decomposition which factors a pair of matrices as a product of unitary and upper triangular matrices. Computing a QZ decomposition is a standard first step when computing generalized eigenvectors, so our algorithm can been seen as a direct simplification of GEVD.

Index Terms—Tensors, CPD, QZ, GEVD, Multilinear Algebra

I. INTRODUCTION

Tensors, or multiindexed numerical arrays, are higher order generalizations of matrices and are natural structures for expressing data and signals which have inherent higher order structure. In this article we study the canonical polyadic decomposition (CPD) which expresses a tensor as a sum of rank one components. The CPD plays an important role in many applications due to the fact that, with mild assumptions, a low rank tensor has a unique CPD [1]–[3]. As such, one can recover underlying component information by computing a CPD of a low rank signal tensor [4]–[6]. The essential uniqueness of CPD has helped make tensors and tensor methods common place in machine learning and signal processing [4], [5].

A standard approach for computing a CPD of a low rank tensor is to first algebraically approximate the decomposition, then to refine the approximation with optimization routines. These algebraic approximations play an important role in optimization routines, as they are relatively inexpensive to compute and the strong initializations they provide can both improve final accuracy and reduce total computation time. Notably, computing a best low rank approximation of a noisy low rank signal tensor is nonconvex and NP-hard [7], so good algebraic initializations greatly aid in getting reliable solutions.

A common approach for algebraic CPD computation is to first compute the generalized eigenvectors of a matrix subpencil of a tensor [8]–[11]. One of the tensor’s factors can then be obtained by computing the inverse transpose of the matrix of generalized eigenvectors for the pencil. This generalized eigenvalue decomposition (GEVD) has been examined by many authors, e.g., see [10]–[12].

We present a simplification of the GEVD algorithm which is more accurate than the original algorithm. As it turns out, the generalized eigenvector computation in GEVD is not needed. Instead, one need only compute a generalized Schur decomposition of a subpencil of the tensor. This decomposition is also called the QZ decomposition. For a generic low rank tensor, the computed Q and Z will simultaneously upper triangularize all frontal slices of the tensor. Our key observation is that, once one has upper triangularized all frontal slices of the tensor, one can simply read off one of the tensors factor matrices from the diagonal entries of the upper triangular slices. Borrowing the perspective of [13], upper triangularizing the frontal slices of a low rank tensor reveals its “joint generalized eigenvalues.”

Computing a QZ decomposition is a standard first step in computing generalized eigenvectors [14], so our algorithm can be seen as a direct simplification of GEVD. Intuitively, we view CPD computation as a (joint) generalized eigenvalue computation rather than a (joint) generalized eigenvector computation. The increase in accuracy of our algorithm is due to the fact that computing the QZ decomposition only relies on unitary matrices as opposed to the general invertible matrices needed for generalized eigenvectors. Furthermore, the QZ method eliminates an inverse computation needed by GEVD.

It is worth noting that ours is not the first algorithm for CPD computation based on simultaneous upper triangularization of the frontal slices of a tensor. For example, in [15] frontal slices are jointly upper triangularized by minimizing the Frobenius norm of the lower triangular portion of the slices. However, the method used in [15] to obtain factor matrices after simultaneous upper triangularization is more involved.

Our QZ based CPD algorithm is presented in Section II. In Section III we prove that our algorithm successfully computes the CPD of a generic low rank tensor. The article ends with Section IV where we illustrate the performance of our algorithm on direction-of-arrival retrieval and in a fluorescence data experiment using the amino acid data set from [16].

Notation and terminology. Let K denote either R or C. We
denote scalars, vectors, matrices, and tensors by lower case ($a$), bold lower case ($\mathbf{a}$), bold upper case ($\mathbf{A}$), and calligraphic script ($\mathcal{A}$), respectively. For a matrix $\mathbf{A} \in \mathbb{R}^{I \times J}$, we let $\mathbf{A}^T$ denote the transpose of $\mathbf{A}$ while $\mathbf{A}^\dagger$ denotes the conjugate transpose of $\mathbf{A}$. If $\mathbf{A}$ is invertible, then we let $\mathbf{A}^{-1}$ denote the inverse of $\mathbf{A}^T$. We use $D_r(\mathbf{A})$ to denote the diagonal matrix whose diagonal entries are given by the $r$th row of $\mathbf{A}$. We say a matrix is generic if it lies in a full measure set. Roughly speaking, a matrix is generic with probability equal to one.

A tensor is a multindexed array with entries in $\mathbb{K}$. The order of a tensor is the number of indices. Given a collection nonzero vectors $\mathbf{u}^{(1)} \in \mathbb{K}^{I_1}, \ldots, \mathbf{u}^{(N)} \in \mathbb{K}^{I_N}$, let

$$u^{(1)}_1 \otimes \cdots \otimes u^{(N)}_N \in \mathbb{K}^{I_1 \times \cdots \times I_N}$$

denote the $I_1 \times \cdots \times I_N$ tensor with mode-$\ell$ unfolding factor matrix $u^{(\ell)}_i$. A tensor of this form is called a rank one tensor. The minimal integer $R$ such that

$$T = \sum_{r=1}^{R} u^{(1)}_r \otimes \cdots \otimes u^{(N)}_r$$

where each $u^{(n)}_r$ has entries in $\mathbb{K}$ is called the $\mathbb{K}$-rank of the tensor $T$, and a decomposition of this form is called a canonical polyadic decomposition (CPD) of $T$. Compactely we write $T = [U^{(1)}, U^{(2)}, \ldots, U^{(N)}]$. Here the matrix $U^{(n)} \in \mathbb{K}^{I_n \times R}$ has $u^{(n)}_r$ as its $r$th column. The matrix $U^{(n)}$ is called a factor matrix of $T$.

A mode-$\ell$ fiber of a tensor is a vector obtained by fixing all indices but the $\ell$th. Defined for a third order tensor, the mode-$\ell$ unfolding $T_{[\ell;i,j]}$ of $T$ is the matrix obtained by stacking all mode-$\ell$ fibers of $T$ as columns of a matrix, where the mode $j$ indices increment faster than the mode-$j$ indices. The $\ell$-mode product $T \cdot A$ between a matrix $A$ and a tensor $T$ is the tensor with mode-$\ell$ unfolding equal to $AT_{[\ell;i,j]}$. We also make use of more general unfoldings for tensors of order greater than three. E.g., if $T \in \mathbb{K}^{I_1 \times I_2 \times I_3}$, then $T_{[4:3:2;1]}$ is an $I_1 I_2 \times I_3$ matrix with $I_1(i_2-1) + i_1, I_3(i_4-1) + i_3$ entry equal to $I_1 i_2 i_3 i_4 i_{i_4}$. We often consider order three subtensors of a tensor. Given a tensor $T \in \mathbb{K}^{I_1 \times \cdots \times I_N}$ and an integer $3 \leq n \leq N$ define

$$T[n] := T(:, ; 1, \ldots, 1; ; 1, \ldots, 1)$$

where the third : occurs in the $n$th mode of $T$. That is, $T[n]$ is an order three subtensor of $T$ formed by fixing all but the first, second, and $n$th. In the case that $T$ has order 3, we call the matrices $\{t(:, ; k)\}_{k=1}^{I_3}$ the frontal slices of $T$.

## II. CPD BY QZ

We now present the CPDQZ algorithm. We let $\mathcal{M} \in \mathbb{K}^{I_1 \times \cdots \times I_N}$ denote a measured tensor of interest, and we assume that $\mathcal{M}$ has the form $\mathcal{M} = T + \mathcal{N}$ where $T$ is the signal portion of $\mathcal{M}$ and where $\mathcal{N}$ is noise. A standard assumption for generalized eigenvalue based algorithms such as GEVD and the generalized eigenspace decomposition (GESD), see [17], is that the tensor $T$ has at least two factor matrices with full column rank. In particular, letting $R$ denote the rank $T$, one has $R \leq \min\{I_1, I_2\}$ up to a permutation of indices. Thus, by computing a (truncated) orthogonal compression of $\mathcal{M}$ such as a multilinear singular value decomposition, see e.g. [18], we can restrict to the case where $\mathcal{M}$ has rank $R$ and size $R \times R \times R_3 \times \cdots \times R_N$ with $R \geq R_\ell$ for all $n$.

When compared to GEVD, our algorithm requires one additional mild assumption. Namely, we assume that the matrix $U^{(N)} \otimes \cdots \otimes U^{(3)}$ has full column rank. Here $\odot$ denotes the Khatri-Rao product. In the upcoming CPDQZS variation of our algorithm, one instead must make the stronger assumption that there is an index $3 \leq n \leq N$ such that $R_n = R$ and $U^{(n)}$ is invertible. These deterministic assumptions are satisfied for generic factor matrices provided the matrices in question all have at least as many rows as columns (before orthogonal compression).

The key observation behind CPDQZ is that one may compute all but two factor matrices of a tensor using a single QZ decomposition together with $n$-mode products. In particular, given a rank $R$ tensor $T \in \mathbb{K}^{R \times R \times R_3 \times \cdots \times R_N}$ which satisfies our assumptions, to obtain factor matrices $U^{(n)}$ for $n \geq 3$, one need only compute unitary matrices $Q$ and $Z$ such that

$$Q T[3](; ; ; 1) Z = Q T[3](; ; ; 2) Z$$

is a QZ decomposition of the matrix pencil

$$(T[3](; ; ; 1), T[3](; ; ; 2)),$$

i.e., such that these matrices are both upper triangular.

Define $T_{qz} := T_{1:} Q Z^T$. It is then a matter of technical formula manipulation to show that

$$U^{(n)}(r, :) = t_{qz}(n)(r, :)$$

for all $n = 3, \ldots, N$ and all $r = 1, \ldots, R$. See the supplementary materials for details.

It remains to compute $U^{(1)}$ and $U^{(2)}$. To do this we first compute $U^{(2)} \odot U^{(1)}$ by solving the overdetermined system

$$T_{[N-1;1,\ldots,1;3;2;1]} = U^{(N)} \odot \cdots \odot U^{(3)} U^{(2)} U^{(1)} T.$$
then computing rank-1 approximations of the appropriately reshaped columns of this matrix. We call the first approach CPDQZ and the second CPDQZS (ingle). For emphasis, CPDQZ and CPDQZS are the same for order three tensors.

For tensors or order greater than three, the difference between these methods is that the CPDQZS method uses rank-1 tensor approximations to compute most of its factors, while the CPDQZ relies more heavily on the initial QZ decomposition to obtain factors. Since a best rank-1 tensor approximation can often be accurately computed and since there is less opportunity for error accumulation before rank-1 tensor approximations are employed in CPDQZS, the CPDQZ method is expected to be more accurate than CPDQZ. This expectation is supported by our numerical experiments.

The growth rate of the cost of both GEVD and CPDQZ is \( O(R^3(\Pi_{i=3}^N R_i)) \). The growth rate of the cost of CPDQZS is \( O(R^4(\Pi_{i=3}^N R_i)) \). If \( R_N = R \), then these growth rates coincide. However, the coefficients of the costs for the methods can be very different. The algorithms all share a step whose cost grows at \( O(R^4(\Pi_{i=3}^N R_i)) \). CPDQZS and GEVD each have additional steps with this growth rate, while CPDQZ does not. Thus, the coefficient of the cost of CPDQZ is lower than that of GEVD or CPDQZS. In practice, CPDQZ is observed to be much faster than CPDQZS and GEVD, see Section IV. See the supplementary materials for further discussion.

III. ALGORITHM DERIVATION

We now derive the CPDQZ algorithm. To ease exposition, we temporarily assume \( T \in \mathbb{R}^{R \times R \times R} \) has order three. The first observation used in the derivation of the CPDQZ algorithm is that in the special case where \( T = [U^{(1)}, U^{(2)}, U^{(3)}] \) has upper triangular frontal slices and meets our assumptions, then in an appropriate column ordering, the matrix \( U^{(1)} \) is upper triangular while the matrix \( U^{(2)} \) is lower triangular.

This fact follows quickly from the main observation behind GEVD. Namely, if \( U^{(1)} \) and \( U^{(2)} \) are \( R \times R \) invertible matrices, then the columns of the matrix \( (U^{(2)})^{-T} \) are equal to the generalized eigenvectors of the matrix pencil

\[
(T(:,1), T(:,2)).
\]

In the case that \( T(:,1) \) and \( T(:,2) \) are upper triangular, a routine argument shows that the pencil’s generalized eigenvectors can be ordered so that \( (U^{(2)})^{-T} \) is upper triangular, hence \( U^{(2)} \) is lower triangular. Having shown that \( U^{(2)} \) is lower triangular, one may use the assumption that \( T \) has upper triangular frontal slices together with the formula

\[
T(:,r) = U^{(1)} D_r (U^{(3)}) (U^{(2)})^T \quad \text{for } r = 1, \ldots, R \quad (1)
\]

to conclude not only that \( U^{(1)} \) is upper triangular, but also that, up to scaling, one has

\[
U^{(3)}(:,r) = \text{diag}(T(:,r)) \quad \text{for } r = 1, \ldots, R.
\]

From this point we need only show that if \( T = [U^{(1)}, U^{(2)}, U^{(3)}] \in \mathbb{R}^{R \times R \times R} \) is an arbitrary tensor which meets our assumptions and if \( Q \) and \( Z \) are matrices which give a QZ decomposition of the matrix pencil

\[
(QT(:,1)Z, QT(:,2)Z),
\]

then the tensor \( T \cdot QZ^T = [QU^{(1)}, Z^T U^{(2)}, U^{(3)}] \) has upper triangular frontal slices. As we shall explain, this fact follows from repeating preceding argument.

Our assumptions guarantee that the pencil \( (T(:,1), T(:,2)) \) has real generalized eigenvalues \([11] \), hence \( QT(:,1)Z \) and \( QT(:,2)Z \) are upper triangular by definition of the QZ factorization and the matrix of generalized eigenvectors of this pencil, i.e., the inverse transpose of the second factor matrix of the tensor \( T \cdot QZ^T \), can be taken to be upper triangular, e.g., see \([14]\). That is, \( Z^T U^{(2)} \) can be taken to be lower triangular.

Applying equation (1) to \( T \cdot QZ^T \) shows that \( QU^{(1)} \) is upper triangular and that all frontal slices of this tensor are upper triangular. Since \( T \) and \( T \cdot QZ^T \) have the same third factor matrix it then easily follows that the CPDQZ algorithm successfully recovers the CPD of a tensor which meets the assumptions stated at the beginning of Section II.

The extension of CPDQZ and CPDQZS to tensors of order greater than three follows a routine argument using the fact that an order \( N \) tensor with CPD \([U^{(1)}, U^{(2)}, \ldots, U^{(N)}]\) can be reshaped to an order three tensor with CPD \([U^{(1)}, U^{(2)}, U^{(3)}] \otimes \cdots \otimes U^{(3)}\).

IV. EXPERIMENTS

The proposed QZ methods make different trade-offs with respect to accuracy and speed. In this section, we compare both methods with the classical GEVD algorithm and the more recent GESD algorithm \([19]\). We use a machine with an AMD Ryzen 5 5600H CPU at 3.30GHz and 16GB of RAM using MATLAB R2021b and Tensorlab 3.0 \([20]\).

In a first experiment, we generate fourth-order low-rank tensors \( T \) by sampling the entries of factor matrices \( A, B, C \) and \( D \) of dimensions \( 80 \times R \) from the uniform distribution on \([0, 1]\) and we normalize all columns to unit length. The rank \( R \) is varied in the range \([4, 16]\) and Gaussian noise is added such that the SNR is 40 dB. For the estimated factor matrices \( \hat{A}, \hat{B}, \hat{C} \) and \( \hat{D} \), we show maximal relative factor matrix errors compared to the true factors, defined as

\[
\max \left( \frac{\|A - \hat{A}\|_F}{\|A\|_F}, \frac{\|B - \hat{B}\|_F}{\|B\|_F}, \frac{\|C - \hat{C}\|_F}{\|C\|_F}, \frac{\|D - \hat{D}\|_F}{\|D\|_F} \right),
\]

where columns of \( \hat{A}, \hat{B}, \hat{C} \) and \( \hat{D} \) have been optimally permuted and scaled to match the columns of \( A, B, C \) and \( D \), respectively. The results are shown in the top plots of Figure 1. CPDQZ is the fastest method, but is less accurate compared to CPDQZS and GEVD. CPDQZS is as fast as GEVD, but is more accurate over the whole range of ranks. In the bottom plots of Figure 1, the experiment is repeated, but now the SNR is varied between 10 and 60 dB, with the rank \( R = 10 \) fixed. The same relative performance is seen for the four methods.

In a more applied experiment, the QZ approach is compared to GEVD in a direction-of-arrival (DOA) retrieval experiment for line-of-sight signals impinging on a uniform rectangular array (URA). The CPD can be applied to find the DOAs in this case \([21]-[23]\). The URA has \( M \times M \) sensors, where \( M = 20 \), and collects \( K = 20 \) samples from \( R = 8 \) far-field sources. These have azimuths \([15 20 25 30 35 40 50 55]\) and elevations
The QZ methods make different trade-offs with respect to time and accuracy. Over 50 trials, CPDQZ (blue) is the fastest, but least accurate, while GESD (red) is the most accurate and the slowest. CPDQZS (green) and GEVD (cyan) are equally fast, but the former is more accurate. The relative performance of the methods for the fourth-order tensors is consistent over varying ranks (with SNR 40 dB) and SNRs (with rank $R = 10$). In both cases, CPDQZS is on average about 8 dB more accurate than GEVD.

We presented the novel CPDQZ and CPDQZS algorithms for algebraic CPD computation which can be viewed as direct simplifications of the popular GEVD algorithm. These algorithms replace the generalized eigenvector computation of GEVD with a QZ decomposition which is used to upper triangularize the frontal slices of a tensor. One factor matrix is then obtained by reading the diagonal entries of the upper triangular slices. We showed in experiments that, in the case of CPDQZS, this simplification results in an increase in accuracy when compared to GEVD. For tensors of order four or more\textsuperscript{4}, CPDQZ is observed to be less accurate but faster than GEVD.

\textsuperscript{4}Recall that CPDQZ and CPDQZS are identical for tensors of order three.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{The QZ methods make different trade-offs with respect to time and accuracy. Over 50 trials, CPDQZ (blue) is the fastest, but least accurate, while GESD (red) is the most accurate and the slowest. CPDQZS (green) and GEVD (cyan) are equally fast, but the former is more accurate. The relative performance of the methods for the fourth-order tensors is consistent over varying ranks (with SNR 40 dB) and SNRs (with rank $R = 10$). In both cases, CPDQZS is on average about 8 dB more accurate than GEVD.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig2.png}
\caption{CPDQZS estimates the elevations of the sources more accurately than GEVD outside of a small SNR window. In addition, CPDQZS has a lower computational cost. Left: mean relative errors over the eight sources of the azimuths (blue) and elevations (green) that are estimated for CPDQZS and the azimuths (red) and elevations (black) that are estimated for GEVD. Right: computation time for both methods. Medians over 500 trials are shown.}
\end{figure}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig3.png}
\caption{The accuracy of CPDQZS (blue) for the estimation of the amino acid concentrations is at least as good as GEVD (cyan) and GESD (red), while requiring a lower computation time. The theoretical emission loading for the three amino acids in function of the wavelength is shown in the left plot. In the center plot, the mode-1 factor matrix error is shown, which corresponds to the estimated concentrations of the amino acids in the five mixtures. The right plot shows the computation times. All results are medians over 100 trials.}
\end{figure}

The relative mode-1 factor matrix errors are shown in the center plot of Figure 3, while the computation times are shown in the right plot. CPDQZS is about as accurate as GEVD and GESD over the range of SNRs and is also notably faster.

\section{Conclusion}

We presented the novel CPDQZ and CPDQZS algorithms for algebraic CPD computation which can be viewed as direct simplifications of the popular GEVD algorithm. These algorithms replace the generalized eigenvector computation of GEVD with a QZ decomposition which is used to upper triangularize the frontal slices of a tensor. One factor matrix is then obtained by reading the diagonal entries of the upper triangular slices. We showed in experiments that, in the case of CPDQZS, this simplification results in an increase in accuracy when compared to GEVD. For tensors of order four or more\textsuperscript{4}, CPDQZ is observed to be less accurate but faster than GEVD.

In future work we will investigate a deflation style algorithm in the spirit of GESD where the deflation step is based on a QZ computation rather than generalized eigenspace computations.

\textsuperscript{4}Recall that CPDQZ and CPDQZS are identical for tensors of order three.
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