ACCELERATING ALTERNATING LEAST SQUARES FOR TENSOR DECOMPOSITION BY PAIRWISE PERTURBATION∗

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Abstract. The alternating least squares algorithm for CP and Tucker decomposition is dominated in cost by the tensor contractions necessary to set up the quadratic optimization subproblems. We introduce a novel family of algorithms that uses perturbative corrections to the subproblems rather than recomputing the tensor contractions. This approximation is accurate when the factor matrices are changing little across iterations, which occurs when alternating least squares approaches convergence. We provide a theoretical analysis to bound the approximation error. Our numerical experiments demonstrate that the proposed pairwise perturbation algorithms are easy to control and converge to minima that are as good as alternating least squares. The performance of the new algorithms shows improvements of 1.3-2.8X with respect to state of the art alternating least squares approaches for various model tensor problems and real datasets on 1, 16 and 256 Intel KNL nodes of the Stampede2 supercomputer.

Key words. tensor, CP decomposition, Tucker decomposition, alternating least squares, tensor condition number

AMS subject classifications. 15A69, 15A72, 65F35, 65K10, 65Y20, 65Y04, 65Y05, 68W25

1. Introduction. Tensor decompositions provide general techniques for approximation and modeling of high dimensional data [11,14,18,20,32,42]. They are fundamental in methods for computational chemistry [9,25,27], physics [39], and quantum information [26,39]. Tensor decompositions are performed on tensors arising both in the context of numerical-PDEs (e.g., as part of preconditioners [41]) as well as in data-driven statistical modeling [3,32,35,36]. The alternating least squares (ALS) method, which is most commonly used to compute many of these tensor decompositions, has become a target for parallelization [22,29], performance optimization [12,46], and acceleration by randomization [8]. We propose a new algorithm that asymptotically accelerates ALS iteration complexity for CP and Tucker decomposition by leveraging an approximation that is provably accurate for well-conditioned problems and is increasingly so as the algorithm approaches the optimization local minima.

Generally, ALS solves quadratic optimization subproblems for individual factors composing the decomposition. It does so in an alternating manner, updating every factor at each sweep. For both CP and Tucker decomposition, computational cost of each sweep is dominated by the tensor contractions needed to setup the quadratic optimization subproblem for every factor matrix. These contractions are redone at every ALS sweep since they involve the factor matrices, all of which change after each sweep. We propose to circumvent these contractions in the scenario when the factor matrices are changing only slightly at each sweep, which is expected when ALS approaches a local minima. Our method approximates the setup of each quadratic optimization subproblem by computing perturbative corrections due to the change in each factor matrices to the quadratic subproblems used for updating each other factor.

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matrix. To do so, pairwise perturbative operators are computed that propagate the change to each factor matrix to the subproblem needed to update each other factor matrix. Computing these operators costs slightly more than a typical ALS iteration. These operators are then reused to approximately perform more ALS sweeps until the changes to the factor matrices are deemed large, at which point, the pairwise operators are recomputed. Each sweep computed approximately in this way costs asymptotically less than a regular ALS sweep.

For CP decomposition, CP-ALS [11,21] is widely used as it provides high-accuracy for the amount of computation required [32] (although alternatives based on gradient and subgradient descent are also competitive [1]). Within CP-ALS, the computational bottleneck of each iteration involves an operation called the matricized tensor-times Khatri-Rao product (MTTKRP). Similarly, the costliest operation in the ALS-based Tucker decomposition (Tucker-ALS) method is called the tensor times matrix-chain (TTMc) product. For an order $N$ tensor with modes of dimension $s$, perturbative approximated computation of ALS sweeps reduces the cost of that sweep from $O(s^n R)$ to $O(s^2 R)$ for a rank-$R$ CP decomposition and from $O(s^n R)$ to $O(s^2 R^{N-1})$ for a rank-$R$ Tucker decomposition.

To quantify the accuracy of the pairwise perturbation approximated algorithm, in Section 4, we provide an error analysis for both the MTTKRP and TTMc operations. For both operations, we first view the ALS procedure in terms of pairwise updates, pushing updates to least-squares problems of all tensors as soon as any one of them is updated. This reformulation is algebraically equivalent to the original ALS procedure. We can bound the absolute error of the way pairwise perturbation propagates updates to any right-hand side due to changes in any one of the other factor matrices for both MTTKRP in CP and TTMc in Tucker decompositions. To leading order in the magnitude of the change $\epsilon$, (or if restricting attention to order three tensors) the absolute error corresponds to a relative error bound based on a matrix condition number. In addition, for the TTMc operation in Tucker decomposition, we derive a 2-norm relative error bound for the overall right-hand-side (as opposed to updates thereof) of $O(\epsilon^2)$ that holds when the residual of the Tucker decomposition is somewhat less than the norm of the original tensor. Finally, we derive a Frobenius norm error bound of $O(\epsilon^2 (s/R)^{N/2})$ for TTMc, which assumes only that HOSVD [15,49] is performed to initialize Tucker-ALS (which is typical).

In order to evaluate the performance benefit of pairwise perturbation, in Section 5, we compare kernels and full decomposition performance on one and many nodes of an Intel KNL system (Stampede2) of implementations developed using the Cyclops [47] and ScaLAPACK [10] libraries. Our microbenchmark results compare the strong and weak scaling performance of one ALS sweep with the best choice of dimension trees [7,31,43,50]. and the first/restart step, in which the pairwise perturbation operators are calculated, as well as the middle steps, in which the operators are not recalculated, of the pairwise perturbation algorithm. These results show that the middle pairwise perturbation steps are 7.4-17.7X faster than one ALS sweep of the dimension tree algorithm in the weak scaling regime, while computing the pairwise operators takes no more than 2.6X the time of a dimension tree ALS sweep. We then study the performance and numerical behavior of pairwise perturbation for decomposition of synthetic tensors and application datasets. Our experimental results show that pairwise perturbation achieves as low residuals as standard ALS, and achieves typical speed-ups of 1.3-2.8X with respect to state of the art dimension tree based ALS algorithms on 1, 16, and 256 KNL nodes. Our results also show that with the increase of the input tensor size, the performance improvements increase,
confirming the asymptotic cost improvement and indicating the potential of pairwise perturbation in large-scale data analysis.

2. Background. This section first outlines the notation that is used throughout this paper, then outlines the basic alternating least square algorithms for both CP and Tucker decomposition.

2.1. Notation and Definitions. Our analysis makes use of tensor algebra in both element-wise equations and specialized notation for tensor operations [32]. For vectors, bold lowercase Roman letters are used, e.g., \( \mathbf{x} \). For matrices, bold uppercase Roman letters are used, e.g., \( \mathbf{X} \). For tensors, bold calligraphic fonts are used, e.g., \( \mathcal{X} \). An order \( N \) tensor corresponds to an \( N \)-dimensional array with dimensions \( s_1 \times \cdots \times s_N \). Elements of vectors, matrices, and tensors are denoted in parentheses, e.g., \( \mathbf{x}(i) \) for a vector \( \mathbf{x} \), \( \mathbf{X}(i,j) \) for a matrix \( \mathbf{X} \), and \( \mathcal{X}(i,j,k,l) \) for an order 4 tensor \( \mathcal{X} \). Columns of a matrix \( \mathbf{X} \) are denoted by \( \mathbf{x}_i = \mathbf{X}(:,i) \).

The mode-\( n \) matrix product of a tensor \( \mathcal{X} \in \mathbb{R}^{I_1 \times \cdots \times I_n} \) with a matrix \( \mathbf{A} \in \mathbb{R}^{J \times s_n} \) is denoted by \( \mathcal{X} \times_n \mathbf{A} \), with the result having dimensions \( s_1 \times \cdots \times s_{n-1} \times J \times s_{n+1} \times \cdots \times s_N \). By juxtaposition of tensor \( \mathcal{X} \) and a matrix \( \mathbf{M} \), we denote the mode-\( N \) product with the transpose of the matrix, \( \mathcal{X} \mathbf{M} = \mathcal{X} \times_N \mathbf{M}^T \). Matricization is the process of unfolding a tensor into a matrix. Given a tensor \( \mathcal{X} \) the mode-\( n \) matricized version is denoted by \( \mathbf{X}(n) \in \mathbb{R}^{s_n \times K} \) where \( K = \prod_{m=1,m \neq n}^N s_m \). We generalize this notation to define the unfoldings of a tensor \( \mathcal{X} \) with dimensions \( \prod_{m=1}^N s_m \) into an order \( M+1 \) tensor, \( \mathcal{X}(i_1,\ldots,i_M) \in \mathbb{R}^{s_{i_1} \times \cdots \times s_{i_M} \times K} \), where \( K = \prod_{i \in \{1,\ldots,N\}\setminus\{i_1,\ldots,i_M\}} s_i \), e.g.,

\[
\mathcal{X}(j,k,l,m) = \mathcal{X}(1,3)(j,l,k+(m-1)\cdot s_2).
\]

We use parenthesized superscripts as labels for different tensors, e.g., \( \mathcal{X}^{(1)} \) and \( \mathcal{X}^{(2)} \) are generally unrelated tensors.

The Hadamard product of two matrices \( \mathbf{U}, \mathbf{V} \in \mathbb{R}^{I \times J} \) resulting in matrix \( \mathbf{W} \in \mathbb{R}^{I \times J} \) is denoted by \( \mathbf{W} = \mathbf{U} \odot \mathbf{V} \), where \( \mathbf{W}(i,j) = \mathbf{U}(i,j)\mathbf{V}(i,j) \). The outer product of \( K \) vectors \( \mathbf{u}^{(1)}, \ldots, \mathbf{u}^{(K)} \) of corresponding sizes \( s_1, \ldots, s_K \) is denoted by \( \mathcal{X} = \mathbf{u}^{(1)} \odot \cdots \odot \mathbf{u}^{(K)} \) where \( \mathcal{X} \in \mathbb{R}^{I_1 \times \cdots \times I_K} \) is an order \( K \) tensor. The Kronecker product of vectors \( \mathbf{u} \in \mathbb{R}^I \) and \( \mathbf{v} \in \mathbb{R}^J \) is denoted by \( \mathbf{w} = \mathbf{u} \otimes \mathbf{v} \) where \( \mathbf{w} \in \mathbb{R}^{I \times J} \). For matrices \( \mathbf{A} \in \mathbb{R}^{I \times K} \) and \( \mathbf{B} \in \mathbb{R}^{J \times K} \), their Khatri-Rao product resulting in a matrix of size \( (IJ) \times K \) defined by

\[
\mathbf{A} \odot \mathbf{B} = [\mathbf{a}^{(1)} \otimes \mathbf{b}^{(1)}, \ldots, \mathbf{a}^{(K)} \otimes \mathbf{b}^{(K)}].
\]

2.2. Tensor Norm. The spectral norm of any tensor \( \mathcal{T} \in \mathbb{R}^{\otimes_{i=1}^N s_i} \) is

\[
\|\mathcal{T}\|_2 = \max_{\forall i \in \{2,\ldots,N\}, \mathbf{x}_i \in \mathbb{R}^{s_i}} \|\mathbf{T}(1)\mathbf{x}_2 \odot \cdots \odot \mathbf{x}_N\|_2, \quad \|\mathbf{x}_2\|_2 = \cdots = \|\mathbf{x}_N\|_2 = 1
\]

where \( \mathcal{T} \) is contracted with \( \mathbf{x}_i \) along its \( i \)-th mode. The spectral tensor norm corresponds to the magnitude of the largest tensor singular value [34]. Computing the spectral norm is NP-hard [23], but can usually be done in practice by specialized variants of ALS [17]. The spectral norm invariant under reordering of modes of \( \mathcal{T} \). Lemma 2.1 shows submultiplicativity of this norm for the tensor times matrix product. 

**Lemma 2.1.** Given any tensor \( \mathcal{T} \in \mathbb{R}^{\otimes_{i=1}^N s_i} \) and matrix \( \mathbf{M} \in \mathbb{R}^{s_N \times R} \), if \( \mathbf{V} = \mathcal{T} \mathbf{M} \) then \( \|\mathbf{V}\|_2 \leq \|\mathcal{T}\|_2 \|\mathbf{M}\|_2 \).
Proof. Assume \( \|\mathbf{V}\|_2 > \|\mathbf{T}\|_2 \|\mathbf{M}\|_2 \), then there exist unit vectors \( \mathbf{x}_2, \ldots, \mathbf{x}_N \) such that
\[
\|\mathbf{V}\|_2 = \|\mathbf{V}(1)(\mathbf{x}_2 \circ \cdots \circ \mathbf{x}_N)\|_2 = \|\mathbf{T}(1)(\mathbf{x}_2 \circ \cdots \circ \mathbf{x}_{N-1} \circ \mathbf{M}\mathbf{x}_N)\|_2.
\]
Let \( \mathbf{z} = \mathbf{M}\mathbf{x}_N \), so \( \|\mathbf{z}\|_2 \leq \|\mathbf{M}\|_2 \). We arrive at a contradiction, since
\[
\|\mathbf{T}(1)(\mathbf{x}_2 \circ \cdots \circ \mathbf{x}_{N-1} \circ \mathbf{z})\|_2 \leq \|\mathbf{T}(1)(\mathbf{x}_2 \circ \cdots \circ \mathbf{x}_{N-1} \circ \mathbf{z})\|_2 \|\mathbf{M}\|_2 \|\mathbf{z}\|_2 \leq \|\mathbf{T}\|_2 \|\mathbf{M}\|_2. \]

2.3. CP Decomposition with ALS. The CP tensor decomposition \([21, 24]\) is a higher-order generalization of the matrix singular value decomposition (SVD). The CP decomposition is denoted by
\[
\mathbf{X} \approx \left[ \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)} \right],
\]
where \( \mathbf{A}^{(i)} = [\mathbf{a}^{(i)}_1, \ldots, \mathbf{a}^{(i)}_r] \), and serves to approximate a tensor by a sum of \( R \) tensor products of vectors:
\[
\mathbf{X} \approx \sum_{r=1}^R \mathbf{a}^{(1)}_r \circ \cdots \circ \mathbf{a}^{(N)}_r.
\]
The CP-ALS method alternates among quadratic optimization problems for each of the factor matrices \( \mathbf{A}^{(n)} \), resulting in linear least squares problems for each row,
\[
\mathbf{A}^{(n)}_{\text{new}} \mathbf{P}^{(n)T} \approx \mathbf{X}^{(n)},
\]
where the matrix \( \mathbf{P}^{(n)} \in \mathbb{R}^{I_n \times R} \), where \( I_n = s_1 \times \cdots \times s_{n-1} \times s_{n+1} \times \cdots \times s_N \) is formed by Khatri-Rao products of the other factor matrices,
\[
\mathbf{P}^{(n)} = \mathbf{A}^{(1)} \circ \cdots \circ \mathbf{A}^{(n-1)} \circ \mathbf{A}^{(n+1)} \circ \cdots \circ \mathbf{A}^{(N)}.
\]
These linear least squares problems are often solved via the normal equations \([32]\). We also adopt this strategy here to devise the pairwise perturbation method. The normal equations for the \( n \)th factor matrix are
\[
\mathbf{A}^{(n)}_{\text{new}} \mathbf{\Gamma}^{(n)} \leftarrow \mathbf{X}^{(n)} \mathbf{P}^{(n)},
\]
where \( \mathbf{\Gamma} \in \mathbb{R}^{r \times r} \) can be computed via
\[
\mathbf{\Gamma}^{(n)} = \mathbf{S}^{(1)} \ast \cdots \ast \mathbf{S}^{(n-1)} \ast \mathbf{S}^{(n+1)} \ast \cdots \ast \mathbf{S}^{(N)},
\]
with each \( \mathbf{S}^{(i)} = \mathbf{A}^{(i)T} \mathbf{A}^{(i)} \).

These equations also give the \( n \)th component of the optimality conditions for the unconstrained minimization of the nonlinear objective function,
\[
f(\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}) = \frac{1}{2} \|\mathbf{X} - [\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]\|_F^2,
\]
for which the \( n \)th component of the gradient is
\[
\frac{\partial f}{\partial \mathbf{A}^{(n)}} = \mathbf{G}^{(n)} = \mathbf{A}^{(n)} \mathbf{\Gamma}^{(n)} - \mathbf{X}^{(n)} \mathbf{P}^{(n)} = (\mathbf{A}^{(n)} - \mathbf{A}^{(n)}_{\text{new}}) \mathbf{\Gamma}^{(n)}.
\]
Algorithm 2.1 presents the basic ALS method described above, keeping track of the Frobenius norm of the \( N \) components of the overall gradient to ascertain convergence.
Algorithm 1.1 CP-ALS: ALS procedure for CP decomposition

1: **Input:** Tensor $\mathcal{X} \in \mathbb{R}^{[N]}$, stopping criteria $\varepsilon$
2: Initialize $[\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]$
3: while $\sum_{n=1}^{N} \| \mathbf{G}^{(n)} \|_F > \varepsilon$ do
4:     for $n \in \{1, \ldots, N\}$ do
5:         $\mathbf{G}^{(n)} \leftarrow \mathbf{S}^{(1)} \mathbf{S}^{(n-1)} \mathbf{S}^{(N)}$
6:         $\mathbf{M}^{(n)} \leftarrow \mathbf{X}_{(n)} \mathbf{A}^{(1)} \mathbf{A}^{(n-1)} \mathbf{A}^{(N)}$
7:         $\mathbf{A}^{(n)}_{\text{new}} \leftarrow \mathbf{M}^{(n)} \mathbf{G}^{(n)}$
8:         $\mathbf{G}^{(n)} \leftarrow (\mathbf{A}^{(n)} - \mathbf{A}^{(n)}_{\text{new}}) \mathbf{G}^{(n)}$
9:         $\mathbf{A}^{(n)} \leftarrow \mathbf{A}^{(n)}_{\text{new}}$
10:     end for
11: end while
12: return $[\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]$

The **Matrixized Tensor Times Khatri-Rao Product** or MTTKRP computation $\mathbf{M}^{(n)} = \mathbf{X}_{(n)} \mathbf{P}^{(n)}$ is the main computational bottleneck of CP-ALS [7]. The computational cost of MTTKRP is $\Theta(s^N R)$ if $s_n = s$ for all $n \in \{1, \ldots, N\}$. The tensor contractions necessary for MTTKRP can be amortized across the linear least squares problems necessary for a given ALS sweep (while loop iteration in Algorithm 1.1). With the best choice of dimension trees [7, 31, 43, 50] to calculate problems necessary for a given ALS sweep, the computational complexity is $4s^N R$. The normal equations worsen the conditioning, but are advantageous for CP-ALS, since $\mathbf{G}^{(n)}$ can be computed and inverted in just $O(s^2 R + R^3)$ cost and the MTTKRP can be amortized by dimension trees. If QR is used instead of the normal equations, the product of $\mathbf{Q}$ with the right-hand sides would have the cost $2s^N R$ and would need to be done for each linear least squares problem, increasing the overall leading order cost by a factor of $N/2$. Our pairwise perturbation algorithm amortizes the dominant cost of the computation of $\mathbf{M}^{(n)} = \mathbf{X}_{(n)} \mathbf{P}^{(n)}$ across multiple ALS sweeps.

Algorithm 2.2 Tucker-ALS: ALS procedure for Tucker decomposition

1: **Input:** Tensor $\mathcal{X} \in \mathbb{R}^{[N]}$, decomposition ranks $\{R_1, \ldots, R_N\}$, stopping criteria $\varepsilon$
2: Initialize $[\mathcal{G}; \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]$ using HOSVD
3: while $\| \mathcal{F} \|_F > \varepsilon$ do
4:     for $n \in \{1, \ldots, N\}$ do
5:         $\mathcal{Y} \leftarrow \mathcal{X} \times_1 \mathbf{A}^{(1)} \times_2 \mathbf{A}^{(2)} \times_{n-1} \mathbf{A}^{(n-1)} \times_n \mathbf{A}^{(n-1)} \times_{n+1} \mathbf{A}^{(n+1)} \times_N \mathbf{A}^{(N)}$
6:         $\mathbf{A}^{(n)} \leftarrow R_n$ leading left singular vectors of $\mathbf{Y}_{(n)}$
7:     end for
8: $\mathcal{G}_{\text{new}} \leftarrow \mathcal{X} \times_1 \mathbf{A}^{(1)} \times_2 \mathbf{A}^{(2)} \times_N \mathbf{A}^{(N)}$
9: $\mathcal{F} \leftarrow \mathcal{G}_{\text{new}} - \mathcal{G}$
10: $\mathcal{G} \leftarrow \mathcal{G}_{\text{new}}$
11: end while
12: return $[\mathcal{G}; \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)}]$

2.4. Tucker Decomposition with ALS. In this section we review the ALS method for computing a low-rank Tucker decomposition of a tensor [49]. Tucker decomposition approximates a tensor by a core tensor contracted by orthogonal matrices.
along each mode. The Tucker decomposition is given by

\[ \mathbf{X} \approx \mathbf{G}, \mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(N)} = \mathbf{g} \times_1 \mathbf{A}^{(1)} \times_2 \mathbf{A}^{(2)} \times_N \mathbf{A}^{(N)}. \]

The corresponding element-wise expression is

\[ \mathbf{X}(x_1, \ldots, x_N) \approx \sum_{\{z_1, \ldots, z_N\}} \mathbf{g}(z_1, \ldots, z_N) \prod_{r \in \{1, \ldots, N\}} \mathbf{A}^{(r)}(x_r, z_r). \]

The core tensor \( \mathbf{G} \) is of order \( N \) with dimensions (Tucker ranks) \( R_1 \times \cdots \times R_N \) (throughout error and cost analysis we assume each \( R_n = R \) for \( n \in \{1, \ldots, N\} \)). The matrices \( \mathbf{A}^{(n)} \in \mathbb{R}^{s_n \times R} \) have orthonormal columns.

The higher-order singular value decomposition (HOSVD) \([15, 49]\) computes the leading left singular vectors of each one-mode unfolding of \( \mathbf{X} \), providing a good starting point for the Tucker-ALS algorithm. The classical HOSVD computes the truncated SVD of \( \mathbf{X}^{(n)} \approx \mathbf{U}^{(n)} \mathbf{\Sigma}^{(n)} \mathbf{V}^{(n)T} \) and sets \( \mathbf{A}^{(n)} = \mathbf{U}^{(n)} \) for \( n \in \{1, \ldots, N\} \). The interlaced HOSVD \([19, 51]\) instead computes the truncated SVD of

\[ \mathbf{Z}^{(n)} = \mathbf{U}^{(n)} \mathbf{\Sigma}^{(n)} \mathbf{V}^{(n)T} \quad \text{where} \quad \mathbf{Z}^{(1)} = \mathbf{X} \quad \text{and} \quad \mathbf{Z}^{(n+1)} = \mathbf{\Sigma}^{(n)} \mathbf{V}^{(n)T}. \]

The interlaced HOSVD is cheaper, since the size of each \( \mathbf{Z}^{(n)} \) is \( s^{N-n+1}R_{n-1} \).

The ALS method for Tucker decomposition \([4, 16, 32]\), which is also called the higher-order orthogonal iteration (HOOI), then proceeds by fixing all except one factor matrix, and computing a low-rank matrix factorization to update that factor matrix and the core tensor. To update the \( n \)th factor matrix Tucker-ALS factorizes

\[ \mathbf{Y}^{(n)} = \mathbf{X} \times_1 \mathbf{A}^{(1)T} \times_2 \mathbf{A}^{(2)T} \times_n \mathbf{A}^{(n-1)T} \times_{n+1} \mathbf{A}^{(n+1)T} \times_N \mathbf{A}^{(N)T} \]

into a product of an orthogonal matrix \( \mathbf{A}^{(n)} \) and the core tensor \( \mathbf{G} \), so that \( \mathbf{Y}^{(n)} \approx \mathbf{A}^{(n)} \mathbf{G}^{(n)} \). This factorization can be done by taking \( \mathbf{A}^{(n)} \) to be the \( R_n \) leading left singular vectors of \( \mathbf{Y}^{(n)} \). This Tucker-ALS procedure is given in Algorithm 2.2.

As in previous work \([13, 40]\), our implementation computes these singular vectors by finding the left eigenvectors of the Gram matrix \( \mathbf{W} = \mathbf{Y}^{(n)T} \mathbf{Y}^{(n)} \). Computing the Gram matrix sacrifices some numerical stability, but avoids a large SVD and provides consistency of the signs of the singular vectors across ALS sweeps.

The Tensor Times Matrix-chain or TTMc computes each \( \mathbf{Y}^{(n)} \) and is the main computational bottleneck of Tucker-ALS \([30]\). With the use of dimensions trees \([7, 31, 43, 50]\) to calculate \( \mathbf{Y}^{(n)} \) in one ALS sweep, the computational complexity for each while loop iteration in Algorithm 2.2 to leading order in \( s \) is \( 4s^N R \).

3. Pairwise Perturbation Algorithms. We now introduce a pairwise perturbation (PP) algorithm to accelerate the ALS procedure when the iterative optimization steps are approaching a local minimum. We first focus on deriving the approximation that asymptotically reduces the cost complexity, then in Section 3.3, provide algorithms that minimize constant factors in cost via dimension trees \([7, 31, 43, 50]\). The key idea of the pairwise perturbation method is to compute pairwise perturbation operators, which correlate a pair of factor matrices. These tensors are then used to repeatedly update the quadratic subproblems for each tensor. As we will show, these updates are provably accurate if the factor matrices do not change significantly since their state at the time of formation of the pairwise perturbation operators.
3.1. CP-ALS. The pairwise perturbation procedure for CP decomposition approximates $M^{(n)} = M^{(n)}$ (defined in Section 2.3) using pairwise perturbation operators $M^{(i,n)}$ for $i \in \{1, \ldots, n-1, n+1, \ldots, N\}$. Below, we define these and more general partially contracted MTTKRP intermediates.

**Definition 3.1.** $M^{(i_1,i_2,\ldots,i_m)}$ is defined as follows,

$$M^{(i_1,i_2,\ldots,i_m)} = X_{(i_1,i_2,\ldots,i_m)} \bigodot_{j=1,\ldots,N\setminus\{i_1,\ldots,i_m\}} A^{(j)}.$$  

Element-wise, we have $M^{(i_1,i_2,\ldots,i_m)}(x_{i_1}, x_{i_2}, \ldots, x_{i_m}, k) = \sum_{\{x_{i_1}, \ldots, x_N\}\setminus\{x_{i_1}, x_{i_2}, \ldots, x_{i_m}\}} X(x_1, \ldots, x_N) \prod_{r \in \{1, \ldots, N\}\setminus\{i_1, i_2, \ldots, i_m\}} A^{(r)}(x_r, k)$.  

Let $A^{(n)}_p$ denote the $A^{(n)}$ calculated with a regular ALS step, some number of steps prior to the current one. Then $A^{(n)}$ at the current step can be expressed as

$$A^{(n)} = A^{(n)}_p + dA^{(n)},$$

and $M^{(n)}$ can be expressed as

$$M^{(n)} = X_{(n)} \bigodot_{i=1,i\neq n} (A^{(i)}_p + dA^{(i)}).$$

The expression above can be rewritten as a function of $M^{(i_1,i_2,\ldots,i_m)}_p$, which is defined in the same way as $M^{(i_1,i_2,\ldots,i_m)}$ except that $X$ is contracted with $A^{(j)}_p$ for $j \in \{1, \ldots, N\}\setminus\{i_1, i_2, \ldots, i_m\}$. $M^{(n)}$ can be expressed as follows,

$$M^{(n)}(y, k) = M^{(n)}_p(y, k) + \sum_{i=1,i\neq n}^{N} \sum_{x=1}^{s_i} M^{(i,n)}_p(x, y, k) dA^{(i)}(x, k) + \sum_{i=1,i\neq n}^{N} \sum_{j=i+1}^{N} \sum_{x=1}^{s_i} \sum_{z=1}^{s_j} M^{(i,j,n)}_p(x, z, y, k) dA^{(i)}(x, k) dA^{(j)}(z, k) + \cdots.$$  

From the above expression we observe that except the first two terms, all terms include the contraction between tensor $M^{(i_1,i_2,\ldots,i_m)}_p$ and at least two matrices $dA^{(i)}$, which are small in norm when each $dA^{(i)}$ is small in norm. The pairwise perturbation algorithm obtains an effective approximation by computing only the first two terms (these terms are described by Figure 1):

$$M^{(n)}(y, k) = M^{(n)}_p(y, k) + \sum_{i=1,i\neq n}^{N} \sum_{x=1}^{s_i} M^{(i,n)}_p(x, y, k) dA^{(i)}(x, k),$$

where $M^{(n)}_p = X_{(n)} \bigodot_{i=1,i\neq n} A^{(i)}_p$, and $M^{(i,n)}_p = X_{(i,n)} \bigodot_{j\in\{1,\ldots,N\}\setminus\{i,n\}} A^{(j)}_p$.  

| State of the art ALS | PP operator construction | PP middle steps |
|----------------------|-------------------------|-----------------|
| CP 4s^R             | 6s^R                    | 2Ns^R          |
| Tucker 4s^R         | 6s^R                    | 2Ns^R          |
Given $M^{(i,n)}_p$ and $M^{(n)}_p$, calculation of $M^{(n)}$ for $n \in \{1, \ldots, N\}$ requires $2Ns^2R$ operations overall. Further, we show in Section 4.1 that the column-wise relative approximation error of $\tilde{M}^{(n)}$ with respect to $M^{(n)}$ is small if each $||d_{a_{kn}}^{(n)}||_2$ for $n \in \{1, \ldots, N\}, k \in \{1, \ldots, R\}$ is sufficiently small. Algorithm 3.1 presents the PP-CP-ALS method described above.

**Algorithm 3.1 PP-CP-ALS:** Pairwise perturbation procedure for CP-ALS

1. **Input:** tensor $\mathcal{X} \in \mathbb{R}^{I_1 \times \cdots \times I_{s_i}}$, stopping criteria $\varepsilon$, PP tolerance $\epsilon$
2. Initialize $[A^{(1)}, \ldots, A^{(N)}]$
3. while $\sum_{i=1}^N ||G^{(i)}||_F > \varepsilon$ do
   4. if $\forall i \in \{1, \ldots, N\}, ||dA^{(i)}||_F < \epsilon$ then
      5. Compute $M^{(i,n)}_p, M^{(n)}_p$ for $i, n \in \{1, \ldots, N\}$ via dimension tree
      6. for $n \in \{1, \ldots, N\}$ do
          7. $A^{(n)}_p \leftarrow A^{(n)}, dA^{(n)} \leftarrow 0$
      8. end for
   9. while $\sum_{i=1}^N ||G^{(i)}||_F > \varepsilon$ and $\forall i \in \{1, \ldots, N\}, ||dA^{(i)}||_F < \epsilon$ do
      10. for $n \in \{1, \ldots, N\}$ do
          11. $\Gamma^{(n)} \leftarrow S^{(1)} \ast \cdots \ast S^{(n-1)} \ast S^{(n+1)} \ast \cdots \ast S^{(N)}$
          12. $\tilde{M}^{(n)}(y,k) = M^{(n)}(y,k) + \sum_{i=1, i \neq n}^N \sum_{x=1}^s M^{(i,n)}_p(x,y,k) dA^{(i)}(x,k)$
          13. $A^{(n)}_{\text{new}} \leftarrow \tilde{M}^{(n)} \Gamma^{(n)^T}$
          14. $G^{(n)} \leftarrow (A^{(n)} - A^{(n)}_{\text{new}}) \Gamma^{(n)}$
          15. $A^{(n)} \leftarrow A^{(n)}_{\text{new}}$
          16. $S^{(n)} \leftarrow A^{(n)T} A^{(n)}$
          17. $dA^{(n)} = A^{(n)}_{\text{new}} - A^{(n)}$
      18. end for
   19. end while
20. end if
21. Perform regular ALS sweep as in Algorithm 2.1, taking $dA^{(n)} \leftarrow A^{(n)}_{\text{new}} - A^{(n)}$ for each $n \in \{1, \ldots, N\}$
22. end while
23. return $[A^{(1)}, \ldots, A^{(N)}]$

3.2. Tucker-ALS. We derive a similar pairwise perturbation algorithm for Tucker ALS. We now seek to approximate $\mathcal{Y}^{(n)} \approx \mathcal{Y}^{(n)}$ (defined in Section 2.4), by forming and reusing pairwise perturbation operators, which are special cases of the following TTMC intermediates.

**Definition 3.2.** $\mathcal{Y}^{(i_1,i_2,\ldots,i_m)}$ is defined as follows,

$$\mathcal{Y}^{(i_1,i_2,\ldots,i_m)} = \mathcal{X} \times_{j \in \{1,\ldots,N\}\setminus\{i_1,i_2,\ldots,i_m\}} A^{(j)T}. \tag{1}$$

Where $\mathcal{X}$ is contracted with all the matrices $A^{(j)}$ without $A^{(i_1)}, \ldots, A^{(i_m)}$.

Similar to the expression for $M^{(n)}$ in CP-ALS, $\mathcal{Y}^{(n)}$ can be expressed as

$$\mathcal{Y}^{(n)} = \mathcal{X} \times_{i=1}^N (A^{(i)T}_p + dA^{(i)T}). \tag{2}$$

The expression above can be rewritten as a function of $\mathcal{Y}^{(i_1,i_2,\ldots,i_m)}_p$, which is defined
in the same way as $\mathbf{Y}^{(i_1, i_2, \ldots, i_m)}$ except that $\mathbf{X}$ is contracted with $A_p^{(j)}$ for $\mathbf{Y}_p^{(i_1, i_2, \ldots, i_m)}$,

$$\mathbf{Y}^{(n)} = \mathbf{Y}_p^{(n)} + \sum_{i=1, i \neq n}^{N} \mathbf{Y}_p^{(n)} \times_i dA^{(i)}T + \sum_{i=1, i \neq n}^{N} \sum_{j=i+1, j \neq n}^{N} \mathbf{Y}_p^{(i, j, n)} \times_i dA^{(i)}T \times_j dA^{(j)}T + \ldots$$

The pairwise perturbation again takes only the first order terms in $dA^{(i)}$, computing

$$\hat{\mathbf{Y}}^{(n)} = \mathbf{Y}_p^{(n)} + \sum_{i=1, i \neq n}^{N} \mathbf{Y}_p^{(n)} \times_i dA^{(i)}T,$$

where $\mathbf{Y}_p^{(n)} = \mathbf{X} \times_{i=1, i \neq n}^{N} A_p^{(i)}T$, and $\mathbf{Y}_p^{(i, n)} = \mathbf{X} \times_{j \in \{1, \ldots, N\} \setminus \{i, n\}} A_p^{(j)}T$.

Given $\mathbf{Y}_p^{(i, n)}$ and $\mathbf{Y}_p^{(n)}$, $\hat{\mathbf{Y}}^{(n)}$ for $n \in \{1, \ldots, N\}$ can be calculated with $2Ns^2R^{N-1}$ cost overall. In Section 4.2, we show that the relative Frobenius norm approximation error of $\hat{\mathbf{Y}}^{(n)}$ with respect to $\mathbf{Y}^{(n)}$ is small, so long as each $\frac{\|dA^{(n)}\|_F}{\|A^{(n)}\|_F}$ is sufficiently small. Algorithm 3.2 presents the PP-Tucker-ALS method described above.

**Algorithm 3.2 PP-Tucker-ALS**: Pairwise perturbation procedure for Tucker-ALS

1: **Input**: tensor $\mathbf{X} \in \mathbb{R}^{r_1 \times \ldots \times r_n}$, decomposition ranks $\{R_1, \ldots, R_N\}$, stopping criteria $\epsilon$, PP tolerance $\epsilon$  
2: Initialize $[\mathbf{G}; A^{(1)}, \ldots, A^{(N)}]$ using HOSVD  
3: while $\|\mathbf{F}\|_F > \epsilon$ do  
4:   if $\forall i \in \{1, \ldots, N\}$, $\|dA^{(i)}\|_F < \epsilon$ then  
5:      Compute $\mathbf{Y}_p^{(i, n)}, \mathbf{Y}_p^{(n)}$ for $i, n \in \{1, \ldots, N\}$ via dimension tree  
6:   for $n \in \{1, \ldots, N\}$ do  
7:      $A_p^{(n)} \leftarrow A^{(n)}, dA^{(n)} \leftarrow O$  
8:   end for  
9: while $\|\mathbf{F}\|_F > \epsilon$ and $\forall i \in \{1, \ldots, N\}$, $\|dA^{(i)}\|_F < \epsilon$ do  
10:   for $n \in \{1, \ldots, N\}$ do  
11:      $\mathbf{Y} \leftarrow \mathbf{Y}_p^{(n)} + \sum_{i=1, i \neq n}^{N} \mathbf{Y}_p^{(i, n)} \times_i dA^{(i)}$  
12:      $A^{(n)} \leftarrow R_n$ leading left singular vectors of $\mathbf{Y}(n)$  
13:      $dA^{(n)} \leftarrow A^{(n)} - A_p^{(n)}$  
14:      $\mathbf{G}_{new} \leftarrow \mathbf{X} \times_1 A^{(1)}T \ldots \times_N A^{(N)}T$  
15:      $\mathbf{F} \leftarrow \mathbf{G}_{new} - \mathbf{F}$  
16:      $\mathbf{G} \leftarrow \mathbf{G}_{new}$  
17:   end for  
18: end while  
19: end if  
20: Perform regular ALS sweep as in Algorithm 2.4, taking $dA^{(n)} \leftarrow A_{new}^{(n)} - A^{(n)}$ for each $n \in \{1, \ldots, N\}$  
21: end while  
22: return $[\mathbf{G}; A^{(1)}, \ldots, A^{(N)}]$  

### 3.3. Dimension Trees for Pairwise Perturbation Operators

Computation of the pairwise perturbation operators $\mathcal{M}_p^{(i, n)}$ and of $\mathcal{M}_p^{(n)}$ can benefit from amortization of common tensor contraction (Khatri-Rao product or tensor-times-matrix product) subexpressions. In the context of ALS, this technique is known as
The main goal of the dimension tree is to perform a minimal number of contractions to obtain each $\mathcal{M}_p^{(i,n)}$. Each matrix $\mathcal{M}_p^{(n)}$ can be simply obtained by a contraction with $\mathcal{M}_p^{(i,n)}$ for any $i \neq n$. Each level of the tree for $l = 1, \ldots, N - 1$ should contain intermediate tensors containing $N - l + 1$ uncontracted modes belonging to the original tensor (the root is the original tensor $\mathbf{X} = \mathcal{M}^{(1,\ldots,N)}$). It’s necessary to maintain the invariant that for any pair of the original tensor modes, each level should contain an intermediate for which these modes are uncontracted. Since the leaves at level $l = N - 1$ have two uncontracted modes, they will include each $\mathcal{M}_p^{(i,n)}$ for $i < n$ ($\mathcal{M}_p^{(i,n),T} = \mathcal{M}_p^{(n,i)}$). At level $l$ it then suffices to compute $\binom{l + 1}{2}$ tensors $\mathcal{M}^{(i,j,l+2,l+4,\ldots,N)}$, $\forall i, j \in \{1, \ldots, l + 2\}, i < j$. Each $\mathcal{M}^{(i,j,l+3,l+4,\ldots,N)}$ can be computed by contraction of $\mathcal{M}^{(s,t,v,l+3,l+4,\ldots,N)}$ and $\mathbf{A}^{(w)}$ where $\{s, t, v\} = \{i, j, w\}$ with $w = \max_{w \in \{l, \ldots, l+2\} \setminus \{i, j\}}(w)$ and $s < t < v$.

The construction of pairwise perturbation operators for CP decomposition costs
\[
2R \sum_{l=2}^{N-1} \binom{l + 1}{2} s^{N-l+2} = 6s^N R + 12s^{N-1} R + O(s^{N-2} R^2).
\]
The cost to form pairwise perturbation operators for Tucker decomposition is
\[
2 \sum_{l=2}^{N-1} \binom{l + 1}{2} s^{N-l+2} R^{l-1} = 6s^N R + 12s^{N-1} R^2 + O(s^{N-2} R^3).
\]

4. **Error Analysis.** In this section, we formally bound the approximation error of the pairwise perturbation algorithm relative to standard ALS. We show that quadratic optimization problems computed by pairwise perturbation differ only slightly from ALS so long as the factor matrices have not changed significantly since the construction of the pairwise perturbation operators. We also provide relative error bounds for the pairwise perturbation algorithm for tensors that are ‘well-conditioned’ based on a notion of condition number defined in Section 8.
Algorithm 4.1 CP-ALS: Reinterpreted ALS procedure for CP decomposition

1: **Input:** Tensor $\mathbf{X} \in \mathbb{R}^{[1:1]}$, stopping criteria $\varepsilon$
2: Initialize $[A^{(1)}, \ldots, A^{(N)}]$ 
3: for $n \in \{1, \ldots, N\}$ do 
4: $M^{(n)} \leftarrow X^{(n)}(A^{(1)} \odot \cdots \odot A^{(n-1)} \odot A^{(n+1)} \odot \cdots \odot A^{(N)})$ 
5: end for 
6: while $\sum_{i=1}^{N} \|G^{(i)}\|_F > \varepsilon$ do 
7: for $n \in \{1, \ldots, N\}$ do 
8: $\Gamma^{(n)} \leftarrow S^{(i)} \odot \ldots \odot S^{(n-1)} \odot S^{(n+1)} \odot \ldots \odot S^{(N)}$ 
9: $A^{(new)} \leftarrow M^{(n)} \Gamma^{(n)}$ 
10: $\delta A^{(n)} = A^{(new)} - A^{(n)}$ 
11: $G^{(n)} \leftarrow -\delta A^{(n)} \Gamma^{(n)}$ 
12: $A^{(n)} \leftarrow A^{(new)}$ 
13: $S^{(n)} \leftarrow A^{(n)} T A^{(n)}$ 
14: for $m \in \{1, \ldots, N\}, m \neq n$ do 
15: $M^{(m)}(x, k) = M^{(m)}(x, k) + \sum_{y=1}^{s_j} M^{(m,n)}(x, y, k) \delta A^{(n)}(y, k)$ 
16: end for 
17: end for 
18: end while 
19: return $[A^{(1)}, \ldots, A^{(N)}]$

4.1. CP-ALS. To understand the error of pairwise perturbation, we view the ALS procedure for CP decomposition in terms of pairwise updates (Algorithm 4.1), pushing updates to least-squares problems of all tensors as soon as any one of them is updated. This reformulation is algebraically equivalent to Algorithm 2.1, but makes oracle-like use of $M^{(m,n)}$ (Definition 3.1), recomputing which would increase the computational cost. We can bound the error of the way pairwise perturbation propagates any right-hand side $M^{(m)}$ due to changes in any one of the other factor matrices $\delta A^{(n)}$. We define the update $H^{(m,n)}$ in terms of its columns:

$$h_k^{(m,n)}(x) = \sum_{y=1}^{s_j} M^{(m,n)}(x, y, k) \delta a_k^{(n)}(y), \quad \text{where} \quad \delta A^{(n)} = A^{(new)} - A^{(n)}.$$

Based on the definition, the update of each $M^{(m)}$ after an ALS sweep is the summation of $H^{(m,n)}$ expressed as $dM^{(m)} = \sum_{n=1, n \neq m}^{N} H^{(m,n)}$. In Theorem 4.1, we prove that when the column-wise norm of $dA^{(n)} = A^{(n)} - A^{(n)}_p$ relative to the norm of $A^{(n)}$, for $n \in \{1, \ldots, N\}$, is small, the absolute error of column-wise results for $H^{(m,n)}$ calculated from pairwise perturbation with respect to that calculated from exact ALS is also small. Corollary 4.2 provides a simple relative error bound for third-order tensors. Overall, these bounds demonstrate that pairwise perturbation should generally compute updates with small relative error with respect to the magnitude of the perturbation of the factor matrices since the setup of the pairwise operators. However, this relative error can be amplified during other steps of ALS, which are ill-conditioned, i.e., can suffer from catastrophic cancellation (the same would hold for round-off error).

**Theorem 4.1.** If $\epsilon^{(l)}_k = \|d a^{(l)}_k\|_2/\|a^{(l)}_k\|_2 < 1$ for all $l \in \{1, \ldots, N\}$, the pairwise
p perturbation algorithm computes the update $\mathbf{H}^{(1,N)}$ with columnwise error,

$$
\|\mathbf{h}_k^{(1,N)} - \mathbf{h}_k^{(1,N)}\|_2 = O\left(\max_{n \in \{2,\ldots,N-1\}} \left\|\hat{\mathbf{T}} \times \mathbf{a}_k^{(j)}\right\|_2 \left\|\mathbf{a}_k^{(n)}\right\|_2 \varepsilon_k^{(n)} \right)
$$

$$
+ \max_{s,t \in \{2,\ldots,N-1\}, s \neq t} \left(\sum_{j=1}^{N-1} \left\|\mathbf{a}_k^{(j)}\right\|_2 \prod_{j=2}^{N-1} \left\|\mathbf{a}_k^{(j)}\right\|_2 \right)
$$

where $\mathbf{H}^{(1,N)}$ is the update to the matrix $\mathbf{M}^{(1)}$ due to the change $\mathbf{dA}^{(N)}$ performed by a regular ALS iteration, and $\hat{\mathbf{T}} = \mathcal{X} \times \mathcal{Y} \delta \mathbf{a}_k^{(N)}$. Analogous bounds hold for $\mathbf{H}^{(m,n)}$ for any $m, n \in \{1, \ldots, N\}$, $m \neq n$.

**Proof.** The ALS update and approximated update are

$$
\mathbf{h}_k^{(1,N)} = \hat{\mathbf{T}} \times \mathbf{a}_k^{(i)} \quad \text{and} \quad \tilde{\mathbf{h}}_k^{(1,N)} = \hat{\mathbf{T}} \times (\mathbf{a}_k^{(i)} - \mathbf{d} \mathbf{a}_k^{(i)}).
$$

We can expand the error as

$$
\mathbf{h}_k^{(1,N)} - \tilde{\mathbf{h}}_k^{(1,N)} = \sum_{S \subseteq \{2,\ldots,N-1\}, S \neq \emptyset} \hat{\mathbf{T}} \times \mathbf{v}_k^{(i)}, \quad \text{where} \quad \mathbf{v}_k^{(i)} = \begin{cases} -\mathbf{d} \mathbf{a}_k^{(i)} : i \in S \\ \mathbf{a}_k^{(i)} : i \notin S \end{cases}.
$$

Consequently, we can upper-bound the error due to terms with $|S| \geq 2$ by

$$
(2^{N-2} - N + 1) \max_{s,t \in \{2,\ldots,N-1\}, s \neq t} \varepsilon_k^{(s)} \varepsilon_k^{(t)} \left\|\hat{\mathbf{T}}\right\|_2 \left\|\mathbf{a}_k^{(j)}\right\|_2.
$$

The error due to the terms with $|S| = 1$ is

$$
\sum_{j \in \{2,\ldots,N-1\}} \hat{\mathbf{T}} \times \mathbf{v}_k^{(i)}, \quad \text{where} \quad \mathbf{v}_k^{(i)} = \begin{cases} -\mathbf{d} \mathbf{a}_k^{(i)} : i = j \\ \mathbf{a}_k^{(i)} : i \neq j \end{cases}.
$$

We can upper-bound the magnitude of this error using a matrix 2-norm by

$$
(N - 2) \max_{n \in \{2,\ldots,N-1\}} \left\|\hat{\mathbf{T}} \times \mathbf{a}_k^{(i)}\right\|_2 \left\|\mathbf{a}_k^{(n)}\right\|_2 \varepsilon_k^{(n)}.
$$

**Corollary 4.2.** For $N = 3$, using the bounds from the proof of Theorem 4.1, under the same assumptions, we obtain the absolute error bound,

$$
\|\mathbf{h}_k^{(1,3)} - \tilde{\mathbf{h}}_k^{(1,3)}\|_2 \leq \left\|\hat{\mathbf{T}}\right\|_2 \left\|\mathbf{a}_k^{(2)}\right\|_2 \varepsilon_k^{(2)}.
$$

Further, since $\mathbf{h}_k^{(1,3)} = \hat{\mathbf{T}} \mathbf{a}_k^{(2)}$, the relative error is bounded by

$$
\frac{\|\mathbf{h}_k^{(1,3)} - \tilde{\mathbf{h}}_k^{(1,3)}\|_2}{\|\mathbf{h}_k^{(1,3)}\|_2} \leq \kappa(\hat{\mathbf{T}}) \varepsilon_k^{(2)}.
$$

From Theorem 4.1, we can conclude that the relative error in computing any column update $\mathbf{h}_k^{(1,3)}$ is $O(\varepsilon)$ when each $\varepsilon_k^{(i)} \leq \varepsilon \ll 1$ and the correct update is sufficiently large, e.g., for $i = 1$ and $j = N$, $\|\mathbf{h}_k^{(1,N)}\|_2 = \Omega\left(\left\|\hat{\mathbf{T}}\right\|_2 \prod_{i=2}^{N-1} \left\|\mathbf{a}_k^{(i)}\right\|_2\right)$. When this is the case, we can also bound the error to the update to the columns of the right-hand sides $d\mathbf{M}^{(n)}$ formed in ALS, so long as the the sum of the updates $\mathbf{H}^{(m,n)}$ for $m \neq n$ does not shrink too much in norm.
4.2. Tucker-ALS. For Tucker decomposition, the pairwise perturbation approximation satisfies even better bounds than for CP decomposition, due to the orthogonality of the factor matrices. We can not only obtain the similar bound as Theorem 4.1, but also obtain stronger results assuming that either the residual of the Tucker decomposition is bounded (it suffices that the decomposition achieves one digit of accuracy in residual) or that the ratio of rank to dimension is not too large. We demonstrate that

- similar to Algorithm 4.1 and Theorem 4.1, when we view the ALS procedure for Tucker decomposition of equidimensional tensors in terms of pairwise updates, we can bound the error of the way pairwise perturbation propagates updates to any right-hand side \( Y^{(m)} \) due to changes in any one of the other factor matrices \( \delta A^{(n)} \).

We define the update \( J^{(m,n)} \) as:

\[
J^{(m,n)} = Y^{(m,n)} \times_n \delta A^{(n)}, \quad \text{where} \quad \delta A^{(n)} = A^{(n)}_{\text{new}} - A^{(n)}.
\]

The similar columnwise absolute error bound as for MTTKR holds for \( J^{(m,n)} \) when the column-wise 2-norm relative perturbations of the input matrices are bounded by \( O(\epsilon) \) (Theorem 4.3).

- the relative error of \( Y^{(m)} \) for \( m \in \{1, \ldots, N\} \) satisfies the bound of \( O(\epsilon^2) \), so long as the residual of Tucker decomposition is small (Theorem 4.5).

- the relative error of \( Y^{(m)} \) for \( m \in \{1, \ldots, N\} \) is bounded in Frobenius norm by \( O(\epsilon^2) \) for a fixed problem size assuming that HOSVD is performed to initialize Tucker-ALS (Theorem 4.8).

**Theorem 4.3.** If \( \epsilon^{(l)}_k = \|da_k^{(l)}\|_2/\|a_k^{(l)}\|_2 < 1 \) for all \( l \in \{1, \ldots, N\} \), For \( X \in \mathbb{R}^{\otimes N \times s} \), if \( \|da_n^{(n)}\|_2 \leq \epsilon \leq 1 \) for \( n \in \{1, \ldots, N\} \), \( k \in \{1, \ldots, R\} \), the pairwise perturbation algorithm computes update \( J^{(1,N)} \) with error,

\[
\|X^{(1,N)} - J^{(1,N)}\|_2 = O\left( \max_{n \in \{2, \ldots, N-1\}} \left\{ \|\hat{T} \times N \sum_{j=2}^{N-1} a_n^{(j)}\|_2 \|a_n^{(n)}\|_2 \epsilon^{(n)}_n \right\} + \max_{s,t \in \{2, \ldots, N-1\}, s \neq t} \epsilon^{(s)} \epsilon^{(t)} \|\hat{T}\|_2 \prod_{j=2}^{N-1} \|a_j^{(j)}\|_2 \right),
\]

where \( \hat{T} = X \times N \delta a_{1}^{(N)} \), \( j^{(1,N)} = J^{(1,1)}(x, i_2, \ldots, i_N) = J^{(1,N)}(x, i_2, \ldots, i_N) \).

**Proof.** The ALS update and approximated update after a change \( \delta A^{(N)} \) are

\[
j^{(1,N)} = \hat{T} \times N \sum_{j=2}^{N-1} a_n^{(j)} \quad \text{and} \quad j^{(1,N)} = \hat{T} \times N \sum_{j=2}^{N-1} (a_n^{(j)} - da_n^{(j)}).
\]

The error bound proceeds by analogy to the proof of Theorem 4.1. \( \square \)

Using Lemma 2.1, we prove in Lemma 4.4 that after contracting a tensor with a matrix with orthonormal rows, whose row length is higher or equal to the column length, the contracted tensor norm is the same as the original tensor norm.

**Lemma 4.4.** Given tensor \( G \in \mathbb{R}^{\otimes n \times r_1} \), the mode-\( n \) product for any \( n \in \{1, \ldots, N\} \), with a matrix with orthonormal columns \( M \in \mathbb{R}^{s \times r_n} \), \( r_n \leq s \), satisfies \( \|G\|_2 = \|G \times_n M\|_2 \).

**Proof.** Based on the submultiplicative property of the tensor norm (Lemma 2.1),

\[
\|G\|_2 = \|G \times (M^T M)\|_2 = \|G \times M \times M^T\|_2 \leq \|G \times M\|_2 \|M^T\|_2 \leq \|G \times M\|_2,
\]

and simultaneously, \( \|G \times M\|_2 \leq \|G\|_2 \|M\|_2 \leq \|G\|_2. \) \( \square \)
Using Lemma 4.4, we prove in Theorem 4.5 that when the relative error of the matrices $A^{(n)}$ for $n \in \{1, \ldots, N\}$ is small and the residual of the Tucker decomposition is loosely bounded, the relative error bound for the $Y^{(n)}$ is independent of the tensor condition number defined in Section 8.

**Theorem 4.5.** Given tensor $\mathbf{X} \in \mathbb{R}^{\otimes_N = 1^{s_1}}$, if $\|dA^{(n)}\|_2 \leq \epsilon \ll 1$ for $n \in \{1, \ldots, N\}$ and $\|\mathbf{X} - [\mathbf{g}; A^{(1)}, A^{(2)}, \ldots, A^{(N)}]\|_2 \leq \frac{1}{3}\|\mathbf{X}\|_2$, $Y^{(n)}$ is constructed with error,

$$\frac{\|\bar{Y}^{(n)} - Y^{(n)}\|_2}{\|Y^{(n)}\|_2} = O(\epsilon^2).$$

**Proof.**

$$\frac{\|\bar{Y}^{(n)} - Y^{(n)}\|_2}{\|Y^{(n)}\|_2} = \left(\frac{N}{2}\right) \max_{i,j} \frac{\|\mathbf{y}^{(i,j,n)} \times_i dA^{(i)T} \times_j dA^{(j)T}\|_2}{\|\mathbf{Y}^{(n)}\|_2} \leq \left(\frac{N}{2}\right) \max_{i,j} \frac{\|\mathbf{y}^{(i,j,n)}\|_2 \|dA^{(i)}\|_2 \|dA^{(j)}\|_2}{\|\mathbf{Y}^{(n)}\|_2}.$$

Let $\bar{\mathbf{X}} = [\mathbf{g}; A^{(1)}, A^{(2)}, \ldots, A^{(N)}]$, $\mathbf{R} = \mathbf{X} - \bar{\mathbf{X}}$. Define the tensors $Z^{(i,j,n)}$ by contraction of $\mathbf{R}$ with all except three factor matrices,

$$Z^{(i,j,n)} = \mathbf{R} \times_r A^{(r)T}.$$

For $\|\mathbf{X} - \bar{\mathbf{X}}\|_2 = \|\mathbf{R}\|_2 \leq \frac{1}{3}\|\mathbf{X}\|_2$, we have $\frac{2}{3}\|\mathbf{X}\|_2 \leq \|\bar{\mathbf{X}}\|_2 \leq \frac{4}{3}\|\mathbf{X}\|_2$. Based on Lemma 4.4,

$$\|Y^{(n)}\|_2 = \|\mathbf{g} \times_n A^{(n)} + Z^{(i,j,n)} \times_i A^{(i)T} \times_j A^{(j)T}\|_2 \geq \|\mathbf{g}\|_2 - \|Z^{(i,j,n)}\|_2 \|A^{(i)T}\|_2 \|A^{(j)T}\|_2 \geq \|\mathbf{g}\|_2 - \|\mathbf{R}\|_2 \geq \frac{1}{3}\|\mathbf{X}\|_2.$$

Additionally,

$$\|Y^{(i,j,n)}\|_2 = \|\mathbf{g} \times_i A^{(i)} \times_j A^{(j)} \times_n A^{(n)} + Z^{(i,j,n)}\|_2 \leq \|\mathbf{g}\|_2 + \|\mathbf{R}\|_2 \leq \frac{5}{3}\|\mathbf{X}\|_2.$$

Therefore,

$$\frac{\|\bar{Y}^{(n)} - Y^{(n)}\|_2}{\|Y^{(n)}\|_2} \leq \left(\frac{N}{2}\right) \max_{i,j} \frac{\|\mathbf{y}^{(i,j,n)}\|_2 \|dA^{(i)}\|_2 \|dA^{(j)}\|_2}{\|\mathbf{Y}^{(n)}\|_2} \leq \left(\frac{N}{2}\right) \frac{2}{3}\|\mathbf{X}\|_2 \epsilon^2 \leq O(\epsilon^2). \quad \Box$$

We now derive a Frobenius norm error bound that is independent of residual norm and tensor condition number, but is looser based on a power the ratio of the tensor dimensions and the Tucker rank. We arrive at this result (Theorem 4.8) by obtaining a lower bound on the residual achieved by the HOSVD (Lemmas 4.6 and 4.7).

**Lemma 4.6.** Given tensor $\mathbf{X} \in \mathbb{R}^{\otimes_N = 1^{s_1}}$ and matrix $A \in \mathbb{R}^{R \times s_n}$, where $R < s_n$ and $A$ consists of $R$ leading left singular vectors of $X^{(n)}$. Let $\mathbf{g} = \mathbf{X} \times_n A$, $\|\mathbf{g}\|_F \geq \|\mathbf{g}\|_F \geq \sqrt{\frac{R}{s_n}} \|\mathbf{X}\|_F$. 

**Proof.** The singular values of $AX^{(n)}$ are the first $R$ singular values of $X^{(n)}$. Since the square of the Frobenius norm of a matrix is the sum of the squares of the singular values, $\|\mathbf{g}\|_F^2 = \|AX^{(n)}\|_F^2 \geq (R/s_n)\|X^{(n)}\|_F^2 = (R/s_n)\|\mathbf{X}\|_F^2$ and $\|\mathbf{g}\|_F \leq \|\mathbf{X}\|_F$. \quad \Box
Lemma 4.7. For any $\mathbf{X} \in \mathbb{R}^{\otimes_{i=1}^{N} s}$, $\|\mathbf{Y}^{(n)}\|_F \geq \left(\frac{R}{s}\right)^{N/2}\|\mathbf{X}\|_F$ if Tucker-ALS starts from an interlaced HOSVD.

Proof. In Tucker-ALS, $\|\mathbf{G}\|_F$ is strictly increasing after each Tucker iteration, where $\mathbf{G}$ is $\mathbf{X}$’s HOSVD core tensor. Since the interlaced SVD computes each $\mathbf{A}^{(n)}$ from the truncated SVD of the product of $\mathbf{X}$ and the first $n-1$ factor matrices, we can apply Lemma 4.6 $N$ times,

$$
\|\mathbf{X} \times_1 \mathbf{A}^{(1)^T} \cdots \times_{N-1} \mathbf{A}^{(N-1)^T}\|_F \geq \|\mathbf{G}\|_F \geq \sqrt{\frac{R}{s}} \|\mathbf{X} \times_1 \mathbf{A}^{(1)^T} \cdots \times_{N-1} \mathbf{A}^{(N-1)^T}\|_F \\
\vdots \\
\|\mathbf{X}\|_F \geq \|\mathbf{G}\|_F \geq \left(\frac{R}{s}\right)^{N/2}\|\mathbf{X}\|_F.
$$

Theorem 4.8. Given tensor $\mathbf{X} \in \mathbb{R}^{\otimes_{i=1}^{N} s}$, if $\|d\mathbf{A}^{(n)}\|_F \leq \epsilon$ for $n \in [1, N]$, $\tilde{\mathbf{Y}}^{(n)}$ is constructed with error,

$$
\frac{\|\tilde{\mathbf{Y}}^{(n)} - \mathbf{Y}^{(n)}\|_F}{\|\mathbf{Y}^{(n)}\|_F} = O\left(\epsilon^2 \left(\frac{s}{R}\right)^{N/2}\right),
$$

assuming that HOSVD is used to initialize Tucker-ALS and the residual associated with factor matrices $\mathbf{A}^{(1)}, \ldots, \mathbf{A}^{(n)}$ is no higher than that attained by HOSVD.

Proof.

$$
\frac{\|\tilde{\mathbf{Y}}^{(n)} - \mathbf{Y}^{(n)}\|_F}{\|\mathbf{Y}^{(n)}\|_F} = \left(\frac{N}{2}\right) \max_{i,j} \frac{\|\mathbf{Y}_p^{(i,j,n)} \times_i d\mathbf{A}^{(i)^T} \times_j d\mathbf{A}^{(j)^T}\|_F}{\|\mathbf{Y}^{(n)}\|_F}.
$$

From Lemma 4.7, we have

$$
\frac{\|\mathbf{Y}_p^{(i,j,n)} \times_i d\mathbf{A}^{(i)^T} \times_j d\mathbf{A}^{(j)^T}\|_F}{\|\mathbf{Y}^{(n)}\|_F} \leq \frac{\|\mathbf{X}\|_F d\mathbf{A}^{(i)^T} \|_F d\mathbf{A}^{(j)^T}\|_F}{\left(\frac{R}{s}\right)^{N/2}\|\mathbf{X}\|_F}.
$$

Consequently, we can bound the relative error by

$$
\frac{\|\tilde{\mathbf{Y}}^{(n)} - \mathbf{Y}^{(n)}\|_F}{\|\mathbf{Y}^{(n)}\|_F} \leq \left(\frac{N}{2}\right) \left(\frac{s}{R}\right)^{N/2} \max_{i,j} \frac{d\mathbf{A}^{(i)^T}}{\|d\mathbf{A}^{(j)^T}\|_F} = O\left(\epsilon^2 \left(\frac{s}{R}\right)^{N/2}\right).
$$

5. Experiments. We evaluate the performance of the pairwise perturbation algorithms on both synthetic and application datasets. The synthetic experiments enable us to test tensors with known factors and to measure whether the algorithm works. We also consider publicly available tensor datasets and demonstrate the effectiveness of our algorithms on practical problems.

We compare the performance of our own implementations of regular ALS with dimension trees and the pairwise perturbation algorithms. All codes are implemented in C++ using Cyclops Tensor Framework (v1.5.3) [47] for all contractions and leveraging its wrapper for the SeaLAPACK [10] SVD routine. Cyclops is a distributed-memory library for tensor contractions, which leverages MPI for interprocess communication and OpenMP for threading. Cyclops employs the HPTT library [48] for high-performance local transposition.

---

1Our implementations are v1.0.0 of https://github.com/LinjianMa/pairwise-perturbation.
The performance results are collected on the Stampede2 supercomputer Texas Advanced Computing Center located at the University of Texas at Austin. We leverage the Knight’s Landing (KNL) nodes exclusively, each of which consists of 68 cores, 96 GB of DDR RAM, and 16 GB of MCDRAM. These nodes are connected via a 100 Gb/sec fat-tree Omni-Path interconnect. We use Intel compilers and the MKL library for threaded BLAS routines within Cyclops, including batched BLAS routines, which are efficient for Khatri-Rao products in CP decomposition. We use 8 processes per node and 8 threads per process for all experiments. While this configuration does not use all cores/threads of Stampede2, it generally provided the best or nearly the best performance rate across different node counts. We do not use the sparse tensor functionality in Cyclops, all storage and computation assumes the tensors are dense.

![Diagram](image)

Figure 2. Benchmark results for ALS sweeps, taken as the mean time across 5 iterations.

5.1. Microbenchmark Results. We first consider a parallel scaling analysis to compare the simulation time for one ALS sweep of the dimension tree algorithm and the restart step and approximated step of the pairwise perturbation algorithm. The pairwise perturbation restart step include the construction of the pairwise perturbation operators, and is therefore much slower than the approximated (middle) steps. For strong scaling, we consider order $N = 6$ tensors with dimension $s = 50$ and rank $R = 6$ CP and Tucker decompositions. For weak scaling, on $p$ processors, we consider order $N = 6$ tensors with dimension $s = \lceil 32p^{1/6} \rceil$ and rank $R = \lceil 4p^{1/6} \rceil$. 
For weak scaling, Figure 2 shows that with the increase of number of nodes, the step time for all three steps increases. The middle step time of pairwise perturbation is always much faster (7.8 and 10.5 times faster on 1 node and 256 nodes, respectively, compared to the dimension tree based ALS step time) than the other two steps, showing the good scalability of pairwise perturbation. For strong scaling, the figure shows that the middle step time of pairwise perturbation increases with the number of nodes, while the other two step times decrease. The middle PP step is much cheaper computationally and become dominated by communication with increasing node counts, thereby slowing down in step time. For the other two steps, the matrix calculation time will be decreased a lot with the increase of node number, thereby the step time is decreased. Overall, we observe that the potential performance benefit of pairwise perturbation is greater for weak scaling.

5.2. Synthetic Tensor Results. We use three synthetic tensors datasets to test the performance of pairwise perturbation:

1. **Tensors with random collinearity and noise** [8]. We create tensors based on known randomly-generated weight vectors \( \lambda \) and factor matrices \( A^{(n)} \). The weight vector \( \lambda \in \mathbb{R}^R \) has entries drawn uniformly from \([0, 2, 0, 8]\), where \( R \) is the true rank of the tensor. The factor matrices \( A^{(n)} \in \mathbb{R}^{s \times R} \) are randomly generated so that the columns have collinearity defined by matrix \( C \in [0, 0.5, 0.9] \mathbb{R}^s \times \mathbb{R}^R \), so that,

\[
C(i, j) = \frac{\langle a_i^{(n)}, a_j^{(n)} \rangle}{\|a_i^{(n)}\|_2 \|a_j^{(n)}\|_2}.
\]

Higher collinearity corresponds to greater overlap between factors, which makes the original factors harder to recover using CP-ALS [45]. Additionally, we add noise to the tensor. Let \( \mathcal{N} \in \mathbb{R}^{s \times s} \) be a tensor with entries drawn from a uniform random distribution. The tensor we aim to decompose is

\[
\mathbf{X} = \mathbf{X}_{\text{true}} + \eta \left( \frac{\|\mathbf{X}_{\text{true}}\|_2}{\|\mathbf{N}\|_2} \right) \mathbf{N} \quad \text{with} \quad \mathbf{X}_{\text{true}} = \sum_{r=1}^{R} \lambda_r a_r^{(1)} \odot \cdots \odot a_r^{(N)},
\]

where \( \eta \) controls the magnitude of noise. In the experiments, we set \( \eta \) to 0.01.

2. **Compact Laplacian tensors**. We transpose and unfold the Laplacian tensor so

\[
\mathbf{X} = \sum_{k=1}^{d} \text{vec}(I) \odot \cdots \odot \text{vec}(I) \odot \text{vec}(D) \odot \text{vec}(I) \odot \cdots \odot \text{vec}(I).
\]

Consequently, \( \mathbf{X} \) is an order \( d \) equidimensional tensor with CP rank \( d \). We will approximate them with rank 2 CP decomposition.

3. **Tensors made by random matrices**. We create tensors based on known uniformly distributed randomly-generated factor matrices \( A^{(n)} \in [0, 1]^{s \times R} \),

\[
\mathbf{X} = [A^{(1)}, \cdots, A^{(N)}],
\]

In the experiments, we set \( R \) to be the same as the decomposition rank.

We tested the synthetic tensors for CP decomposition. These tensors all have low ranks and are suitable for testing the speed-up from pairwise perturbation. For tensor 1 and tensor 3, on \( p \) processors, we consider order \( N = 6 \) tensors with dimension \( s = [32p^{1/6}] \) and rank \( R = [4p^{1/6}] \). For tensor 2, on \( p \) processors, we consider order \( N = 4 \) tensors with dimension \( s = [169p^{1/4}] \) and rank \( R = 2 \).
We display the relative residual norm and execution time for each CP decomposition problem in Figure 3. We observe that pairwise perturbation achieves a lower execution time for all tensors. For Figure 3a, 3b and 3c, due to the rapid decrease of the residual in the initial steps, we also plot the gradient norm, which controls convergence. Pairwise perturbation performs best for larger tensor sizes, which is consistent with our cost analysis. The speedup for Tensor 1 is 1.5-2.2X, for Tensor 2 is 1.8-2.7X, and for Tensor 3 is 2.0-2.8X. Additionally, different PP restarting tolerance (0.002, 0.01 and 0.05) are shown, which restart the pairwise perturbation scheme when the relative norm difference of each decomposed matrix between two neighboring steps exceeds the tolerance. We can see that for small tensors (shown in Figure 3a, 3d and 3g), a loose tolerance (0.05) can start the pairwise perturbation earlier, leading to relatively better performance. However, when the tensor size is large (shown in Figure 3c and 3i), this loose tolerance (0.05) may lead to the instability of the convergence procedure.
We also note that pairwise perturbation often achieves a lower final residual (most noticeably in Figure 3e). For Figure 3e, the residual norm with tolerance 0.01, 0.05 is 0.53, 0.74 times the residual norm of normal ALS, respectively. This phenomena may be due to the introduction of noise by the perturbative approximation, allowing ALS to find a smaller local minima (similar observations have been made by approximate randomized ALS schemes [8]).

5.3. Tensor Application Dataset Results. We use two application datasets to test the performance benefits of pairwise perturbation:

1. **COIL Data Set.** COIL-100 is an image-recognition data set that contains images of objects in different poses [38] and has been used previously as a tensor decomposition benchmark [8, 52]. There are 100 different object classes, each of which is imaged from 72 different angles. Each image has 128 × 128 pixels in three color channels. Transferring the data into tensor format, we have a 128 × 128 × 3 × 7200 tensor. We fix the CP decomposition rank to be 10 and the Tucker decomposition rank to be 10 × 10 × 10 × 3 × 70.

2. **Time-Lapse Hyperspectral Radiance Images.** We consider the 3D hyperspectral imaging dataset called “Souto wood pile” [37]. The dataset is usually used on the benchmark of nonnegative tensor decomposition [6, 33]. The hyperspectral data consists of a tensor with dimensions 1024 × 1344 × 33 × 9. We fix the CP decomposition rank to be 10 and the Tucker decomposition rank to be 100 × 100 × 10 × 5.

We display the relative residual norm and execution time for CP decomposition of the two real datasets in Figure 4a, 4b. We observe that pairwise perturbation achieves a lower execution time for them. The speedup for the Coil Dataset is 1.5-2.0X and for the Time-Lapse Dataset is 2.1-2.5X. Additionally, a larger PP restarting tolerance (0.1) leads to better performance.

Pairwise perturbation is also used to speedup HOOI procedure in Tucker decomposition. However, as noted in other work [5], we observed that ALS iterations do not significantly lower the residual beyond what is achieved by the first iteration (HOSVD). Nevertheless, we study the benefit of pairwise perturbation on reaching convergence of ALS faster (it is possible that a more practical benefit from pairwise perturbation would be achieved for variations of Tucker decomposition that enforce additional constraints or for other tensors).

We display the relative residual norm, the relative norm change of core tensor and execution time for Tucker decomposition of the two real datasets in Figure 4c, 4d. The speedup for the Coil Dataset is 1.02-1.04X and for the Time-Lapse Dataset is 1.11-1.28X. The reason for no obvious speed-up for the Coil Dataset is that the tensor is not equidimensional (one dimension is 7200, while others are all smaller or equal to 128). Therefore, when updating the factor matrix with a dimension of 7200, the number of operations necessary to construct the SVD input for PP are similar to that for the dimension tree Tucker algorithm. For the Time-Lapse Dataset, the tensor dimensions are more evenly distributed (two dimensions are greater than 1000), and we observe a greater speed-up. We conclude that the proposed Tucker PP algorithm performs better when used on the tensors whose dimensions are approximately equal.
Figure 4. Experimental results between pairwise perturbation and dimension tree algorithm for CP and Tucker decompositions on 1 KNL node. Each dot on the dimension tree/PP lines represents the results per 10 ALS iterations for CP and per ALS iteration for Tucker decomposition, and the black circles on pairwise perturbation lines represent the time when pairwise perturbation restarts.

6. Conclusion. We have provided a pairwise perturbation algorithm for both CP and Tucker decompositions for dense tensors. The advantage of this algorithm is that it uses perturbative corrections rather than recomputing the tensor contractions to set up the quadratic optimization subproblems, and is accurate when the factor matrices change little, based on our error analysis. Specifically, our Cyclops implementation of pairwise perturbation shows speed-ups for CP-ALS of 1.5-2.8X across all synthetic and application data with respect to the best known method for exact CP-ALS (also implemented with Cyclops).

We leave analysis and benchmarking of pairwise perturbation with sparse tensors for future work. Since contraction between the input tensor and the first factor matrix will require fewer operations, the benefit of pairwise perturbation is likely to be lesser. Additionally, it is likely of interest to investigate more efficient adaptations of pairwise perturbation for non-equidimensional tensors and to experiment with alternative schemes for switching between regular ALS and pairwise perturbation.

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8. Appendix: Error Bounds based on a Tensor Condition Number. We provide relative error bounds for the pairwise perturbation algorithm for both CP-ALS and Tucker-ALS for tensors that are 'well-conditioned', in a sense that is defined in this appendix. However, results related to the Hurwitz problem regarding multiplicative relations of quadratic forms [28], imply that equidimensional order three tensors can have a bounded condition number only if their dimension is \( s \in \{1, 2, 4, 8\} \). We provide families of tensors with unit condition number with such dimensions. However, for factorization of large tensors, the bounds proven in this section are not meaningful, since their condition number is necessarily infinite for at least one ordering of modes.

8.1. Tensor Condition Number. We consider a notion of tensor condition number that corresponds to a global bound on the conditioning of the multilinear vector-valued function, \( g_\mathcal{T} : \otimes_{i=2}^{N} \mathbb{R}^{s_i} \to \mathbb{R}^{s_1} \) associated with the product of the tensor with vectors along all except the first mode,

\[
g_\mathcal{T}(x_2, \ldots, x_N) = \mathcal{T}(1)(x_2 \circ \cdots \circ x_N),
\]

where \( \mathcal{T} \) is contracted with \( x_1 \) along its 1st mode. The norm and condition number are given by extrema of the norm amplification of \( g_\mathcal{T} \), which are described by the amplification function \( f_\mathcal{T} : \otimes_{i=2}^{N} \mathbb{R}^{s_i} \to \mathbb{R} \),

\[
f_\mathcal{T}(x_2, \ldots, x_N) = \frac{\|g_\mathcal{T}(x_2, \ldots, x_N)\|_2}{\|x_2\|_2 \cdots \|x_N\|_2}.
\]

The spectral norm of the tensor corresponds to its supremum,

\[
\|\mathcal{T}\|_2 = \sup\{f_\mathcal{T}\}.
\]

The tensor condition number is then defined as

\[
\kappa(\mathcal{T}) = \sup\{f_\mathcal{T}\} / \inf\{f_\mathcal{T}\},
\]

which enables quantification of the worst-case relative amplification of error with respect to input for the product of a tensor with vectors along all except the first mode. In particular, \( \kappa(\mathcal{T}) \) provides an upper bound on the relative norm of the perturbation of \( g_\mathcal{T} \) with respect to the relative norm of any perturbation to any input vector.

For a matrix \( \mathbf{M} \in \mathbb{R}^{s_1 \times s_2} \), if \( s_1 > s_2 \) the above notion of condition number gives

\[
\kappa(\mathbf{M}) = \sigma_{\max}(\mathbf{M}) / \sigma_{\min}(\mathbf{M}) \quad \text{where} \quad \sigma_{\min}(\mathbf{M}) \quad \text{is the smallest singular value of} \quad \mathbf{M} \quad \text{in the reduced SVD, while if} \quad s_1 < s_2, \quad \text{then} \quad \kappa(\mathbf{M}) = \infty.
\]

When tensor dimensions are unequal, the condition number is infinite if the first dimension is not the largest, so for some \( i, s_i > s_1 \). Aside from this condition, the ordering of modes of \( \mathcal{T} \) does not affect the condition number, since for any \( m > 1 \), the supremum/infimum of \( f_\mathcal{T} \) over the domain of unit vectors are for some choice of \( x^{(2)}, \ldots, x^{(m-1)}, x^{(m+1)}, \ldots, x^{(N)} \) the maximum/minimum singular values of

\[
\mathbf{K} = \mathcal{T}_{(1,m)}(x^{(2)} \circ \cdots \circ x^{(m-1)} \circ x^{(m+1)} \circ \cdots \circ x^{(N)}).
\]
8.2. Well-Conditioned Tensors. We provide two examples of order three tensors that have unit condition number. Other perfectly conditioned tensors can be obtained by multiplying the above tensors by an orthogonal matrix along any mode (we prove below that such transformations preserve condition number). The first example has \( s = 2 \), and yields a Givens rotation when contracted with a vector along the last mode. It is composed of two slices:

\[
\begin{bmatrix}
1 & 1 \\
-1 & 1
\end{bmatrix}
\]

The second example has \( s = 4 \) and is composed of four slices:

\[
\begin{bmatrix}
1 & 1 \\
1 & -1
\end{bmatrix},
\begin{bmatrix}
-1 & 1 \\
1 & 1
\end{bmatrix},
\begin{bmatrix}
1 & -1 \\
1 & 1
\end{bmatrix},
\begin{bmatrix}
-1 & 1 \\
1 & 1
\end{bmatrix}
\]

Finally, for \( s = 8 \), we provide an example by giving matrices \( M \) and \( N \), so that the tensor has nonzeros \( T(i,j,k) = N(i,j) \) for each entry in \( M \).

\[
M = \begin{bmatrix}
1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 \\
2 & 1 & 4 & 3 & 6 & 5 & 8 & 7 \\
3 & 4 & 1 & 2 & 7 & 8 & 5 & 6 \\
4 & 3 & 2 & 1 & 8 & 7 & 6 & 5 \\
5 & 6 & 7 & 8 & 1 & 2 & 3 & 4 \\
6 & 5 & 8 & 7 & 2 & 1 & 4 & 3 \\
7 & 8 & 5 & 6 & 3 & 4 & 1 & 2 \\
8 & 7 & 6 & 5 & 4 & 3 & 2 & 1
\end{bmatrix},
N = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
-1 & 1 & -1 & 1 & -1 & -1 & -1 & 1 \\
-1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 \\
-1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 \\
-1 & 1 & 1 & -1 & -1 & 1 & 1 & 1 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1 & -1 \\
-1 & -1 & -1 & -1 & -1 & -1 & -1 & -1
\end{bmatrix}.
\]

The fact that the latter two tensors have unit condition number can be verified by symbolic algebraic manipulation or numerical tests.

These tensors provide solutions to special cases of the Hurwitz problem [28], which seeks bilinear forms \( z_1, \ldots, z_n \) in variables \( x_1, \ldots, x_l \) and \( y_1, \ldots, y_m \) such that

\[
(x_1^2 + \cdots + x_l^2)(y_1^2 + \cdots + y_m^2) = z_1^2 + \cdots + z_n^2.
\]

Consequently, if for \( T \) and any vectors \( x, y \),

\[
\frac{\|T \times_2 x \times_3 y\|_2}{\|x\|_2 \|y\|_2} = 1 \quad \Rightarrow \quad \|T \times_2 x \times_3 y\|_2 = \|x\|_2 \|y\|_2,
\]

so we can define bilinear forms,

\[
z_i = \sum_j \sum_k T(i,j,k)x_jy_k,
\]

that provide a solution to the Hurwitz problem. Such equidimensional tensors with unit condition number exist for dimension \( s \in \{1, 2, 4, 8\} \) [44], corresponding to the Hurwitz problem with \( l = m = n = s \). However, solutions to the Hurwitz problem with \( l = m = n \) cannot exist for any other dimension. Furthermore, tight bounds exist on the dimension \( s_3 \) for a tensor of dimensions \( s \times s \times s_3 \) to have bounded condition number (\( \inf \{f_T\} > 0 \)). This problem is equivalent to finding \( s_3 \) matrices of dimension \( s \times s \), such that any nonzero linear combination thereof is invertible. Factorizing \( s = 2^{4a+b+c} \), where \( b \in \{0, 1, 2, 3\} \) and \( c \) is odd, \( s_3 \leq 8a + 2^b \) [2].
8.3. Properties of the Tensor Condition Number. In our analysis, we make use of the following submultiplicativity property of the tensor condition number with respect to tensor times matrix products (the property also generalizes to pairs of arbitrary order tensors contracted over one mode).

**Lemma 8.1.** For any $\mathcal{T} \in \mathbb{R}^{n_1 \times \cdots \times n_s}$ and matrix $M$, if $\mathcal{V} = \mathcal{T}M$ then $\kappa(\mathcal{V}) \leq \kappa(\mathcal{T}) \kappa(M)$.

**Proof.** Assume $\kappa(\mathcal{V}) > \kappa(\mathcal{T})\kappa(M)$, then there exist unit vectors $x_2, \ldots, x_N$ and $y_2, \ldots, y_N$ such that

$$\kappa(\mathcal{T})\kappa(M) < \kappa(\mathcal{V}) = \frac{\|V_1(x_2 \circ \cdots \circ x_N)\|_2}{\|V_1(y_2 \circ \cdots \circ y_N)\|_2} = \frac{\|T_1(x_2 \circ \cdots \circ x_{N-1} \circ Mx_N)\|_2}{\|T_1(y_2 \circ \cdots \circ y_{N-1} \circ My_N)\|_2}.$$  

Let $u = Mx_N$ and $v = My_N$, so $\|u\|_2/\|v\|_2 \leq \kappa(M)$, yielding a contradiction,

$$\kappa(\mathcal{V}) \leq \frac{\|T_1(x_2 \circ \cdots \circ x_{N-1} \circ (u/\|u\|_2))\|_2}{\|T_1(y_2 \circ \cdots \circ y_{N-1} \circ (v/\|v\|_2))\|_2} \kappa(\mathcal{T}) \leq \kappa(\mathcal{T})\kappa(M).$$

Applying Lemma 8.1 with a vector, i.e. when $M \in \mathbb{R}^{N \times 1}$ and so has condition number $\kappa(M) = 1$, implies $\kappa(\mathcal{T}M) \leq \kappa(\mathcal{T})$. By an analogous argument to the proof of Lemma 8.1, we can also conclude that the norm and infimum of such a product of $\mathcal{T}$ with unit vectors are bounded by those of $\mathcal{T}$, giving the following corollary.

**Corollary 8.2.** For any $\mathcal{T} \in \mathbb{R}^{n_1 \times \cdots \times n_s}$, vector $u \in \mathbb{R}^{s_n}$, and any $n \in \{1, \ldots, N\}$ such that $\exists m \in \{1, \ldots, N\}$ with $s_m \geq s_n$ and $m \neq n$, if $\mathcal{V} = \mathcal{T} \times_n u$, then $\|\mathcal{V}\|_2 \leq \|u\|_2/\|\mathcal{T}\|_2\inf\{f_{\mathcal{V}}\} \geq \|u\|_2\inf\{f_{\mathcal{T}}\}$, and $\kappa(\mathcal{V}) \leq \kappa(\mathcal{T})$.

For an orthogonal matrix $M$, Lemma 8.1 can be applied in both directions, namely for $\mathcal{V} = \mathcal{T}M$ and $\mathcal{T} = \mathcal{V}M^T$, so we observe that $\kappa(\mathcal{V}) = \kappa(\mathcal{T})$. Using this fact, we demonstrate in the following theorem that any tensor $\mathcal{T}$ can be transformed by orthogonal matrices along each mode, so that one of its fibers has norm $\|\mathcal{T}\|_2/\kappa(\mathcal{T})$.

**Theorem 8.1.** For any $\mathcal{T} \in \mathbb{R}^{n_1 \times \cdots \times n_s}$, there exist orthogonal matrices $Q_2, \ldots, Q_N$, with $Q_i \in \mathbb{R}^{n_i \times n_i}$, such that $\mathcal{V} = \mathcal{T} \times_2 Q_2 \times_3 \cdots \times_N Q_N$ satisfies $\kappa(\mathcal{V}) = \kappa(\mathcal{T})$, $\|\mathcal{V}\|_2 = \|\mathcal{T}\|_2/\kappa(\mathcal{T})$, and the first fiber of $\mathcal{V}$, i.e. the vector $v$ with $v(i) = V(i, 0, \ldots, 0)$, satisfies $\|v\|_2 = \|\mathcal{T}\|_2/\kappa(\mathcal{T})$.

**Proof.** Given a tensor $\mathcal{T}$ with infinite condition number, there must exist $N - 1$ unit vectors $x_2, \ldots, x_N$, such that $\|T_1(x_2 \circ \cdots \circ x_N)\|_2 = \|\mathcal{T}\|_2/\kappa(\mathcal{T})$. We define $N - 1$ orthogonal matrices $Q_2, \ldots, Q_N$ such that $Q_i^T x_i = e_i$. We can then contract $\mathcal{T}$ with these matrices along the last $N - 1$ modes, resulting in $\mathcal{V}$, with the same condition number as $\mathcal{T}$ (by Lemma 8.1) and the same norm (by a similar argument). Then, we have that the first fiber of $\mathcal{V}$ is

$$v = V_1(e_2 \circ \cdots \circ e_N) = T_1(x_2 \circ \cdots \circ x_N),$$

and consequently $\|v\|_2 = \|\mathcal{T}\|_2/\kappa(\mathcal{T})$. □

By Theorem 8.1, the condition number of a tensor is infinity if and only if it can be transformed by products with orthogonal matrices along the last $N - 1$ modes into a tensor with a zero fiber. Further, any tensor $\mathcal{T}$ may be perturbed to have infinite condition number by adding to it some $\delta \mathcal{T}$ with relative norm $\|\delta \mathcal{T}\|_2/\|\mathcal{T}\|_2 = 1/\kappa(\mathcal{T})$.

8.4. PP-CP-ALS Error Bound using Tensor Condition Number. For CP decomposition, we obtain condition-number-dependent column-wise error bounds
Lemma 8.1 implies that for any \( i, j, k \), the contribution of second order terms to the error is

\[
\| m_k^{(n)} - m_k^{(n)} \|_2 = O(\epsilon^2 k(\mathcal{A})),
\]

where \( M^{(n)} \) is the matrix given by a regular ALS iteration.

**Theorem 8.3.** If \( \frac{\| a_k^{(n)} \|_2}{\| a_k^{(n)} \|_2} \leq \epsilon < 1 \) for \( n \in \{1, \ldots, N\} \), \( k \in \{1, \ldots, R\} \) and \( s_m \leq s_n \) for any \( m \in \{1, \ldots, N\} \), the pairwise perturbation algorithm computes \( \tilde{M}^{(n)} \) with column-wise error,

\[
\frac{\| m_k^{(n)} - m_k^{(n)} \|_2}{\| m_k^{(n)} \|_2} = O(\epsilon^2 k(\mathcal{A})),
\]

and the pairwise perturbation operators \( O \) of \( m_k^{(n)} \) by similar analysis, higher-order perturbations would lead to errors smaller by a factor of \( O(\text{poly}(N)\epsilon) \) and are consequently negligible if \( \epsilon \ll 1 \). Consider the order four tensors \( \mathcal{M}^{(i,j,n)} \) (Definition 3.1) based on the current factor matrices \( A^{(1)}, \ldots, A^{(N)} \) and the pairwise perturbation operators \( \mathcal{M}_p^{(i,j,n)} \) based on past factor matrices \( A_p^{(1)}, \ldots, A_p^{(N)} \). The contribution of second order terms to the error is

\[
m_k^{(n)}(x) - m_k^{(n)}(x) \approx \sum_{i,j \in \{1, \ldots, n-1, n+1, \ldots, N\}} \sum_{y=1}^s \sum_{z=1}^s \mathcal{M}_p^{(i,j,n)}(x, y, z, k) a_k^{(i)}(y) a_k^{(j)}(z).
\]

This absolute error has magnitude,

\[
\| m_k^{(n)}(x) - m_k^{(n)}(x) \|_2 \leq \left( \frac{N}{2} \right) \max_{i,j} \| \mathcal{M}_p^{(i,j,n)}(\cdot, \cdot, \cdot, k) \|_2 \| a_k^{(i)} \|_2 \| a_k^{(j)} \|_2.
\]

Using the fact that for any \( i, j \) we can express \( m_k^{(n)} \) as

\[
m_k^{(n)}(x) = \sum_{y=1}^s \sum_{z=1}^s \mathcal{M}^{(i,j,n)}(x, y, z, k) a_k^{(i)}(y) a_k^{(j)}(z),
\]

we can lower bound the magnitude of the answer with respect to any \( \mathcal{M}^{(i,j,n)} \),

\[
\| m_k^{(n)} \|_2 \geq \inf \{ \| f_{\mathcal{M}^{(i,j,n)}}(\cdot, \cdot, \cdot, k) \|_2 \} \| a_k^{(i)} \|_2 \| a_k^{(j)} \|_2.
\]

Combining the upper bound on the absolute error with the lower bound on norm,

\[
\frac{\| m_k^{(n)} - m_k^{(n)} \|_2}{\| m_k^{(n)} \|_2} \leq \left( \frac{N}{2} \right) \max_{i,j} \| \mathcal{M}_p^{(i,j,n)}(\cdot, \cdot, \cdot, k) \|_2 \| a_k^{(i)} \|_2 \| a_k^{(j)} \|_2.
\]

Lemma 8.1 implies that for any \( i, j, k \),

\[
\| \mathcal{M}_p^{(i,j,n)}(\cdot, \cdot, \cdot, k) \|_2 \leq \| \mathcal{X} \|_2 \prod_{l \in \{1, \ldots, N\} \setminus \{i,j,n\}} \| A_p^{(l)}(\cdot, \cdot, k) \|_2
\]

and that

\[
\inf \{ \| f_{\mathcal{M}^{(i,j,n)}}(\cdot, \cdot, \cdot, k) \|_2 \} \geq \inf \{ \| f_X \|_2 \} \prod_{l \in \{1, \ldots, N\} \setminus \{i,j,n\}} \| A^{(l)}(\cdot, \cdot, k) \|_2
\]
Since, \( \|A_p^{(l)}(:, k)\|_2 \leq (1 + \epsilon)\|A^{(l)}(:, k)\|_2 \), we obtain the bound,
\[
\frac{\|\tilde{m}_k^{(n)} - m_k^{(n)}\|_2}{\|m_k^{(n)}\|_2} \leq \left(\frac{N}{2}\right) \kappa(\mathbf{X})(1 + \epsilon)^{N-3}\epsilon^2 \approx \left(\frac{N}{2}\right) \kappa(\mathbf{X})\epsilon^2. 
\]
This error bound is relative to the condition number of \( \mathbf{X} \), which means the bound is sensitive to the input tensor and that the error may be unbounded if \( \mathbf{X} \) has an exact CP decomposition of rank at most \( \min_i s_i \).

8.5. PP-Tucker-ALS Error Bound using Tensor Condition Number.
For Tucker decomposition, we again obtain bounds based on the perturbation to \( A^{(n)} \), this time for \( Y^{(n)} \) (the tensors on whose matricizations a truncated SVD is performed). Using Lemma 8.1, we prove in Theorem 8.4 that when the tensor has same length in each mode and the relative error of the matrices \( A^{(n)} \) for \( n \in \{1, \ldots, N\} \) is small, the relative error for the \( \tilde{Y}^{(n)} \) is also small.

**Theorem 8.4.** Given tensor \( \mathbf{X} \in \mathbb{R}^{\otimes_{i=1}^N s_i} \), if \( \|dA^{(n)}\|_2 \leq \epsilon \ll 1 \) for \( n \in \{1, \ldots, N\} \), \( \tilde{Y}^{(n)} \) is constructed with error,
\[
\frac{\|Y^{(n)} - \tilde{Y}^{(n)}\|_2}{\|Y^{(n)}\|_2} = O(\epsilon^2 \kappa(\mathbf{X})).
\]

**Proof.** As in Theorem 8.3, we bound the error due to second-order terms,
\[
\frac{\|Y^{(n)} - \tilde{Y}^{(n)}\|_2}{\|Y^{(n)}\|_2} \leq \left(\frac{N}{2}\right) \max_{i,j} \frac{\|Y_p^{(i,j,n)} \times_i dA^{(i)}T \times_j dA^{(j)}T\|_2}{\|Y_p^{(i,j,n)} \times_i A^{(i)}T \times_j A^{(j)}T\|_2}.
\]
From Lemma 8.1, we have
\[
\frac{\|Y_p^{(i,j,n)} \times_i dA^{(i)}T \times_j dA^{(j)}T\|_2}{\|Y_p^{(i,j,n)} \times_i A^{(i)}T \times_j A^{(j)}T\|_2} \leq \frac{\|Y_p^{(i,j,n)}\|_2 \|dA^{(i)}\|_2 \|dA^{(j)}\|_2}{\inf_i \|f_{Y^{(i,j,n)}}\|_2 \|A^{(i)}\|_2 \|A^{(j)}\|_2}.
\]
Since \( A^{(i)} \) and \( A^{(j)} \) are both matrices with orthonormal columns,
\[
\frac{\|Y^{(n)} - \tilde{Y}^{(n)}\|_2}{\|Y^{(n)}\|_2} \leq \left(\frac{N}{2}\right) \max_{i,j} \frac{\|Y_p^{(i,j,n)}\|_2 \|dA^{(i)}\|_2 \|dA^{(j)}\|_2}{\inf_i \|f_{Y^{(i,j,n)}}\|_2} = O(\epsilon^2 \kappa(\mathbf{X})).
\]
\]