

BlockTensorDecompositions.jl: A Unified Constrained Tensor Decomposition Julia Package

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1 Introduction

- Tenors are useful in many applications
- Need tools for fast and efficient decompositions

For the scientific user, it would be most useful for there to be a single piece of software that can take as input 1) any reasonable type of factorization model and 2) constraints on the individual factors, and produce a factorization. Details like what rank to select, how the constraints should

be enforced, and convergence criteria should be handled automatically, but customizable to the knowledgeable user. These are the core specification for `BlockTensorDecompositions.jl`.

1.1 Related tools

- Packages within Julia
- Other languages
- Hint at why I developed this

Beyond the external usefulness already mentioned, this package offers a playground for fair comparisons of different parameters and options for performing tensor factorizations across various decomposition models. There exist packages for working with tensors in languages like Python (TensorFlow [1], PyTorch [2], and TensorLy [3]), MATLAB (Tensor Toolbox [4]), R (rTensor [5]), and Julia (TensorKit.jl [6], Tullio.jl [7], OMEinsum.jl [8], and TensorDecompositions.jl [9]). But they only provide a groundwork for basic manipulation of tensors and the most common tensor decomposition models and algorithms, and are not equipped to handle arbitrary user defined constraints and factorization models.

Some progress towards building a unified framework has been made [10–12]. But these approaches don't operate on the high dimensional tensor data natively and rely on matricizations of the problem, or only consider nonnegative constraints. They also don't provide an all-in-one package for executing their frameworks.

1.2 Contributions

- Fast and flexible tensor decomposition package
- Framework for creating and performing custom
 - tensor decompositions
 - constrained factorization (the what)
 - iterative updates (the how)
- Implement new “tricks”
 - a (Lipschitz) matrix step size for efficient sub-block updates
 - multi-scaled factorization when tensor entries are discretizations of a continuous function
 - partial projection and rescaling to enforce linear constraints (rather than Euclidean projection)
- ?? rank detection ??

The main contribution is a description of a fast and flexible tensor decomposition package, along with a public implementation written in Julia: `BlockTensorDecompositions.jl`. This package provides a framework for creating and performing custom tensor decompositions. To the author's knowledge, it is the first package to provide automatic factorization to a large class of constrained tensor decompositions problems, as well as a framework for implementing new constraints and iterative algorithms. This paper also describes three new techniques not found in the literature that empirically converge faster than traditional block-coordinate descent.

2 Tensor Decompositions

- the math section of the paper

This section reviews the notation used throughout the paper and commonly used tensor decompositions.

2.1 Notation

- tensor notation, use MATLAB notation for indexing so subscripts can be used for a sequence of tensors

2.1.a Sets

The set of real number is denoted as \mathbb{R} and its restrictions to nonnegative numbers is denoted as $\mathbb{R}_+ = \mathbb{R}_{\geq 0} = \{x \in \mathbb{R} \mid x \geq 0\}$.

We use $[N] = \{1, 2, \dots, N\} = \{n\}_{n=1}^N$ to denote integers from 1 to N .

Usually, lower case symbols will be used for the running index, and the capitalized letter will be the maximum letter it runs to. This leads to the convenient shorthand $i \in [I]$, $j \in [J]$, etc.

We use a capital delta Δ to denote sets of vectors or higher order tensors where the slices or fibres along a specified dimension sum to 1, i.e. generalized simplexes.

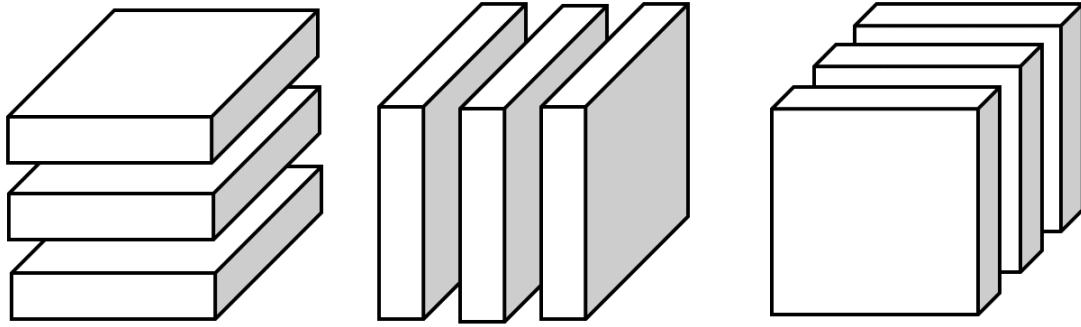
Usually, we use script letters (\mathcal{A} , \mathcal{B} , \mathcal{C} , etc.) for other sets.

2.1.b Vectors, Matrices, and Tensors

Vectors are denoted with lowercase letters (x , y , etc.), and matrices and higher order tensors with uppercase letters (commonly A , B , C and X , Y , Z). The order of a tensor is the number of axes it has. We would call vectors “order-1” or “1st order” tensors, and matrices “order-2” or “2nd order” tensors.

To avoid confusion between entries of a vector/matrix/tensor and indexing a list of objects, we use square brackets to denote the former, and subscripts to denote the later. For example, the entry in the i th row and j th column of a matrix $A \in \mathbb{R}$ is $A[i, j]$. This follows MATLAB/Julia notation where $A[i, j]$ points to the entry $A[i, j]$. We contrast this with a list of I objects being denoted as a_1, \dots, a_I , or more compactly, $\{a_i\}$ when it is clear the index $i \in [I]$.

The n -slices, n th mode slices, or mode n slices of an N th order tensor A are notated with the slice $A[:, \dots, :, i_n, :, \dots, :]$. For a 3rd order tensor A , the 1st, 2nd, and 3rd mode slices $A[i, :, :]$, $A[:, j, :]$, and $A[:, :, k]$ have special names and are called the horizontal, lateral, and frontal slices and are displayed in Figure 1. In Julia, the 1-, 2-, and 3-slices of a third order array A would be `eachslice(A, dims=1)`, `eachslice(A, dims=2)`, and `eachslice(A, dims=3)`.

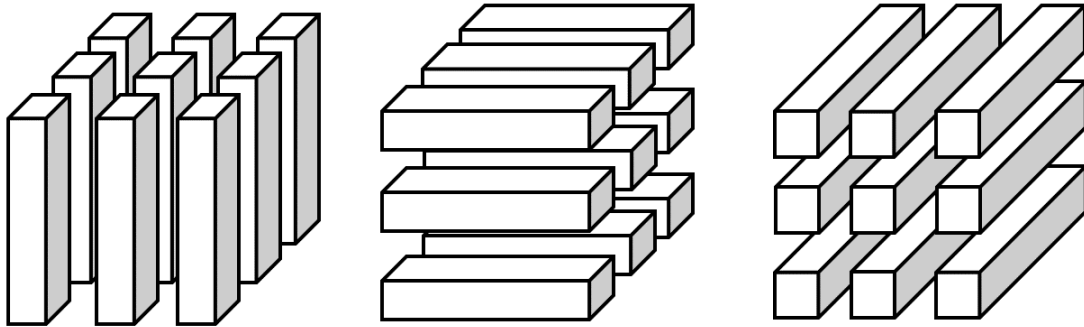


(a) horizontal slices $A[i, :, :]$ (b) lateral slices $A[:, j, :]$ (c) frontal slices $A[:, :, k]$

Figure 1: Slices of an order 3 tensor A .

The n -fibres, n th mode fibres, or mode n fibres of an N th order tensor A are denoted $A[i_1, \dots, i_{n-1}, :, i_{n+1}, \dots, i_N]$. For example, the 1-fibres of a matrix M are the column vectors $M[:, j]$, and the 2-fibres are the row vectors $M[i, :]$. For order-3 tensors, the 1st, 2nd, and 3rd mode fibres $A[:, j, k]$, $A[i, :, :]$, and $A[i, j, :]$ are called the vertical/column, horizontal/row, and depth/tube fibres respectively and are displayed in Figure 2. Natively in Julia, the 1-, 2-, and 3-fibres of a third order array A would be `eachslice(A, dims=(2,3))`, `eachslice(A, dims=(1,3))`, and `eachslice(A, dims=(1,2))`. `BlockTensorDecomposition.jl` defines the function `eachfibre(A; n)` to do exactly this. For example, the 1-fibres of an array A would be `eachfibre(A, n=1)`.

For matrices, the 1-fibres are the same as the 2-slices (and vice versa), but for N th order tensors in general, fibres are always vectors, whereas n -slices are $(N - 1)$ th order tensors.



(a) vertical fibres $A[:, j, k]$ (b) horizontal fibres $A[i, :, k]$ (c) depth fibres $A[i, j, :]$

Figure 2: Fibres of an order 3 tensor A .

Since we commonly use I as the size of a tensor's dimension, we use id_I to denote the identity tensor of size I (of the appropriate order). When the order is 2, id_I is an $I \times I$ matrix with ones along the main diagonal, and zeros elsewhere. For higher orders N , this is an $\underbrace{I \times \dots \times I}_{N \text{ times}}$ tensor where $\text{id}_I[i_1, \dots, i_N] = 1$ when $i_1 = \dots = i_N \in [I]$, and is zero otherwise.

`BlockTensorDecomposition.jl` defines `identity_tensor(I, ndims)` to construct id_I .

2.1.c Operations

The Frobenius inner product between two tensors $A, B \in \mathbb{R}^{I_1 \times \dots \times I_N}$ is denoted

$$\langle A, B \rangle = A \cdot B = \sum_{i_1=1}^{I_1} \dots \sum_{i_N=1}^{I_N} A[i_1, \dots, i_N] B[i_1, \dots, i_N].$$

Julia's standard library package `LinearAlgebra` implements the Frobenius inner product with `dot(A, B)` or `A · B`.

The n -slice dot product \cdot_n between two tensors $A \in \mathbb{R}^{I_1, \dots, I_{n-1}, J, I_{n+1}, \dots, I_N}$ and $B \in \mathbb{R}^{I_1, \dots, I_{n-1}, K, I_{n+1}, \dots, I_N}$ returns a matrix $(A \cdot_n B) \in \mathbb{R}^{J \times K}$ with entries

$$(A \cdot_n B)[j, k] = \sum_{i_1 \dots i_{n-1} i_{n+1} \dots i_N} A[i_1, \dots, i_{n-1}, j, i_{n+1}, \dots, i_N] B[i_1, \dots, i_{n-1}, k, i_{n+1}, \dots, i_N].$$

This product can also be thought of as taking the dot product between all pairs of n th order slices of A and B : $(A \cdot_n B)[j, k] = A_j \cdot B_k$.

`BlockTensorDecomposition.jl` defines this operation with `slicewise_dot(A, B, n)`. In the special case where $A = B$, a more efficient method that only computes entries where $i \leq j$ is defined since $A \cdot_n A$ is a symmetric matrix.

The n -mode product \times_n between a tensor $A \in \mathbb{R}^{I_1 \times \dots \times I_N}$ and matrix $B \in \mathbb{R}^{I_n \times J}$, returns a tensor $(A \times_n B) \in \mathbb{R}^{I_1 \times \dots \times I_{n-1} \times J \times I_{n+1} \times \dots \times I_N}$ with entries

$$(A \times_n B)[i_1, \dots, i_{n-1}, j, i_{n+1}, \dots, i_N] = \sum_{i_n=1}^{I_n} A[i_1, \dots, i_{n-1}, i_n, i_{n+1}, \dots, i_N] B[i_n, j].$$

`BlockTensorDecomposition.jl` defines this operation with `nmode_product(A, B, n)`.

```
function nmode_product(A::AbstractArray, B::AbstractMatrix, n::Integer)
    # convert the problem to the mode-1 product
    Aperm = swapdims(A, n)
    Cperm = Aperm ×₁ B
    return swapdims(Cperm, n) # swap back
end

function ×₁(A::AbstractArray, B::AbstractMatrix)
    # Turn the 1-mode product into matrix-matrix multiplication
    sizeA = size(A)
    Amat = reshape(A, sizeA[1], :)

    # Initialize the output tensor
    C = zeros(size(B)[1], sizeA[2:end]...)
    Cmat = reshape(C, size(B)[1], prod(sizeA[2:end]))

    # Perform matrix-matrix multiplication Cmat = B*Amat
```

```

mul!(Cmat, B, Amat)

return C # Output entries of Cmat in tensor form
end

function swapdims(A::AbstractArray, a::Integer, b::Integer=1)
    # Construct a permutation where a and b are swapped
    # e.g. [4, 2, 3, 1, 5, 6] when a=4 and b=1
    dims = collect(1:ndims(A))
    dims[a] = b; dims[b] = a
    return permutedims(A, dims)
end

```

The Frobenius norm of a tensor A is the square root of its dot product with itself

$$\|A\|_F = \sqrt{\langle A, A \rangle}.$$

For vectors v , this is equivalent to the (Euclidean) 2-norm

$$\|v\|_F = \|v\|_2 = \sqrt{\langle v, v \rangle}.$$

For matrices M , the (Operator) 2-norm is defined as

$$\|M\|_2 = \arg \max_{\|v\|_2=1} \|Mv\|_2 = \sigma_1(M)$$

where $\sigma_1(M)$ is the largest singular value of M .

For tensors T , the (Operator) 2-norm needs to be defined in terms of how we treat them as function on other tensors. There is a canonical way to do this for vectors $x \rightarrow v^\top x$ and matrices $x \rightarrow Mx$, but not tensors. This is relevant to Section 3.2.b where the Lipschitz step-size is computed in terms of the Operator norm of the Hessian of our objective function.

2.2 Common Decompositions

- Extensions of PCA/ICA/NMF to higher dimensions
- talk about the most popular Tucker, Tucker-n, CP
- other decompositions
 - high order SVD (see Kolda and Bader)
 - HOSVD (see Kolda, Shifted power method for computing tensor eigenpairs)

A tensor decomposition is a factorization of a tensor into multiple (usually smaller) tensors, that can be recombined into the original tensor. Computationally, we can think of a generic decomposition as storing factors (A, B, C, \dots) and operations $(\times_a, \times_b, \dots)$ for combining them. This is what we do in `BlockTensorDecomposition.jl`.

```

struct GenericDecomposition{T, N} <: AbstractArray{T, N}
    factors::Tuple{Vararg{AbstractArray{T}}} # e.g. (A, B, C)
end

```

```

    contractions::Tuple{Vararg{Function}} # e.g. (×1, ×2)
end
# Y = A ×1 B ×2 C
array(G::GenericDecomposition) = multifoldl(contractions(G), factors(G))

```

The function `multifoldl` applies the given operations between each factor, from left to right.

```

function multifoldl(ops, args)
    @assert (length(ops) + 1) == length(args)
    x = args[begin]
    for (op, arg) in zip(ops, args[begin+1:end])
        x = op(x, arg)
    end
    return x
end

```

Different types of decompositions define different operations, and different “ranks” of the same decomposition specific the sizes of the factors used.

A commonly used family of decompositions can be derived from the Tucker decomposition.

Definition 2.1: A rank- (R_1, \dots, R_N) Tucker decomposition of a tensor $Y \in \mathbb{R}^{I_1 \times \dots \times I_N}$ produces N matrices $A_n \in \mathbb{R}^{I_n \times R_n}$, $n \in [N]$, and core tensor $B \in \mathbb{R}^{R_1 \times \dots \times R_N}$ such that

$$Y[i_1, \dots, i_N] = \sum_{r_1=1}^{R_1} \dots \sum_{r_N=1}^{R_N} A_1[i_1, r_1] \dots A_N[i_N, r_N] B[r_1, \dots, r_N] \quad (1)$$

entry-wise. More compactly, this decomposition can be written using the n -mode product, or with double brackets

$$Y = B \times_1 A_1 \times_2 \dots \times_N A_N = B \bigtimes_n A_n = \llbracket B; A_1, \dots, A_N \rrbracket.$$

Sometimes we write $A_0 = B$ to ease notation, and suggest the “zeroth” factor of the tucker decomposition is the core tensor B . In the special case when $N = 3$, we can visualize Tucker decomposition as multiplying the core tensor by matrices on all three sides as shown in Figure 3.

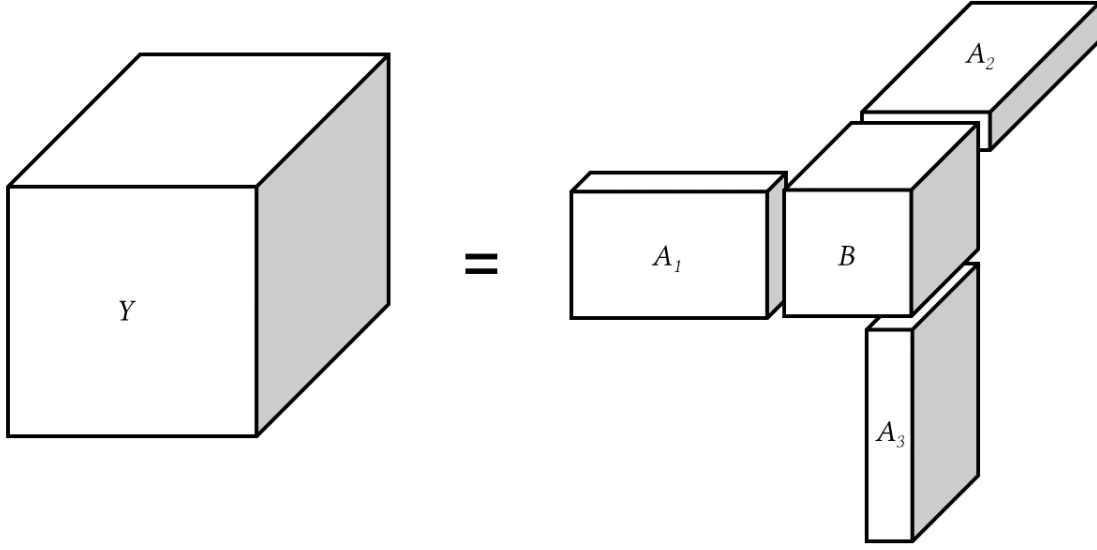


Figure 3: Tucker factorization of a 3rd order tensor Y .

Setting all the matrices of a Tucker decomposition to the identity matrix but the first gives the Tucker-1 decomposition.

Definition 2.2: A rank- R Tucker-1 decomposition of a tensor $Y \in \mathbb{R}^{I_1 \times \dots \times I_N}$ produces a matrix $A \in \mathbb{R}^{I_1 \times R}$, and core tensor $B \in \mathbb{R}^{R \times I_2 \times \dots \times I_N}$ such that

$$Y[i_1, \dots, i_N] = \sum_{r=1}^R A[i_1, r] B[r, i_2, \dots, i_N] \quad (2)$$

entry-wise or more compactly,

$$Y = AB = B \times_1 A = \llbracket B; A \rrbracket.$$

Note we extend the usual definition of matrix-matrix multiplication

$$(AB)[i, j] = \sum_{r=1}^R A[i, r] B[r, j]$$

to tensors B in the compact notation for Tucker-1 decomposition $Y = AB$.

More generally, any number of matrices can be set to the identity matrix giving the Tucker- n decomposition.

Definition 2.3: A rank- (R_1, \dots, R_n) Tucker- n decomposition of a tensor $Y \in \mathbb{R}^{I_1 \times \dots \times I_N}$ produces n matrices A_1, \dots, A_n , and core tensor $B \in \mathbb{R}^{R_1 \times \dots \times R_n \times I_{n+1} \times \dots \times I_N}$ such that

$$Y[i_1, \dots, i_N] = \sum_{r_1=1}^{R_1} \dots \sum_{r_n=1}^{R_n} A_1[i_1, r_1] \dots A_n[i_n, r_n] B[r_1, \dots, r_n, i_{n+1}, \dots, i_N] \quad (3)$$

entry-wise, or compactly written in the following three ways,

$$\begin{aligned} Y &= B \times_1 A_1 \times_2 \dots \times_n A_n \times_{n+1} \text{id}_{I_{n+1}} \times_{n+2} \dots \times_N \text{id}_{I_N} \\ Y &= B \times_1 A_1 \times_2 \dots \times_n A_n \\ Y &= \llbracket B; A_1, \dots, A_n \rrbracket. \end{aligned}$$

Lastly, if we set the core tensor B to the identity tensor id_R , we obtain the **canonical decomposition/parallel factors model** (CANDECOMP/PARAFAC or CP for short).

Definition 2.4: A rank- R CP decomposition of a tensor $Y \in \mathbb{R}^{I_1 \times \dots \times I_N}$ produces N matrices $A_n \in \mathbb{R}^{I_n \times R}$, such that

$$Y[i_1, \dots, i_N] = \sum_{r=1}^R A_1[i_1, r] \dots A_N[i_N, r] \quad (4)$$

entry-wise. More compactly, this decomposition can be written using the n -mode product, or with double brackets

$$Y = \text{id}_R \times_1 A_1 \times_2 \dots \times_N A_N = \text{id}_R \bigtimes_n A_n = \llbracket A_1, \dots, A_N \rrbracket.$$

Note CP decomposition is sometimes referred to as Kruskal decomposition, and requires the core only be diagonal (and not necessarily identity) and the factors A_n have normalized columns $\|A_n[:, r]\|_2 = 1$.

Other factorization models are used that combine aspects of CP and Tucker decomposition [13], are specialized for order 3 tensors [14, 15], or provide alternate decomposition models entirely like tensor-trains [16]. But the (full) Tucker, and its special cases Tucker- n , and CP decomposition are most commonly used extensions of the low-rank matrix factorization to tensors. These factorizations are summarized in Table 1.

Table 1: Summary of common tensor factorizations. Here, N is the order of the factorized tensor.

Name	Bracket Notation	n -mode Product	Entry-wise
Tucker	$\llbracket A_0; A_1, \dots, A_N \rrbracket$	$A_0 \times_1 A_1 \times_2 \dots \times_N A_N$	Equation 1
Tucker-1	$\llbracket A_0; A_1 \rrbracket$	$A_0 \times_1 A_1$	Equation 2
Tucker- n	$\llbracket A_0; A_1, \dots, A_n \rrbracket$	$A_0 \times_1 A_1 \times_2 \dots \times_n A_n$	Equation 3
CP	$\llbracket A_1, \dots, A_N \rrbracket$	$\text{id}_R \times_1 A_1 \times_2 \dots \times_N A_N$	Equation 4

TODO add discussion on other decompositions - high order SVD (see Kolda and Bader) - HOSVD (see Kolda, Shifted power method for computing tensor eigenpairs)

Tensor decompositions are not necessarily unique. It should be clear that scaling one factor by $x \neq 0$ and dividing another by x yields the same original tensor. Furthermore, fibres and slices can be permuted without affecting the the original tensor. Up to these manipulations, for a fixed rank, there exist criteria that ensures their decompositions are unique [13, 17, 18].

2.2.a Representing Tucker Decompositions

There are implemented in `BlockTensorDecomposition.jl` and can be called, for a third order tensor, with `Tucker((B, A1, A2, A3))`, `Tucker1((B, A1))`, and `CPDecomposition((A1, A2, A3))`. These Julia structs store the tensor in its factored form. If the recombined tensor or particular entries are requested, Julia dispatches on the type of decomposition and calls a particular method of `array` or `getindex`. The implementations for efficient array construction and index access are provided below.

```
array(T::Tucker) = multifoldl(tucker_contractions(ndims(T)), factors(T))
tucker_contractions(N) = Tuple{(G, A) -> nmode_product(G, A, n) for n in 1:N}
```

TODO add `getindex` method for Tucker type

```
function array(T::Tucker1)
    B, A = factors(T)
    return B ×1 A
end

function getindex(T::Tucker1, I::Vararg{Int})
    B, A = factors(T)
    i = I[1]
    J = I[begin+1:end] # J = (I2, I3, ..., IN)
    return (@view A[i, :]) · view(B, :, J...)
end
```

```
array(CPD::CPDecomposition) =
    mapreduce(vector_outer, +, zip((eachcol.(factors(CPD)))...))
```

```
vector_outer(v) = reshape(kron(reverse(v)...),length.(v))

getindex(CPD::CPDecomposition, I::Vararg{Int}) =
    sum(reduce(.*, (@view f[i,:]) for (f,i) in zip(factors(CPD), I)))
```

2.3 Tensor rank

- tensor rank
- constrained rank (nonnegative etc.)

The rank of a matrix $Y \in \mathbb{R}^{I \times J}$ can be defined as the smallest $R \in \mathbb{Z}_+$ such that there exists an exact factorization $Y = AB$ for some $A \in \mathbb{R}^{I \times R}$ and $B \in \mathbb{R}^{R \times J}$.

Although this can be extended to higher order tensors, we must specify under which factorization model we are using. For example, the *CP-rank* R of a tensor Y is the smallest such R that admits an exact CP decomposition of Y .

Definition 2.5: The CP rank of a tensor $Y \in \mathbb{R}^{I_1 \times \dots \times I_N}$ is the smallest R such that there exist factors $A_n \in \mathbb{R}^{I_n \times R}$ and $Y = \llbracket A_1, \dots, A_N \rrbracket$,

$$\text{rank}_{\text{CP}}(Y) = \min\{R \mid \exists A_n \in \mathbb{R}^{I_n \times R}, n \in [N] \quad \text{s.t.} \quad Y = \llbracket A_1, \dots, A_N \rrbracket\}$$

In a similar way, we can define the *Tucker-1-rank* R .

Definition 2.6: The Tucker-1 rank of a tensor $Y \in \mathbb{R}^{I_1 \times \dots \times I_N}$ is the smallest R such that there exist factors $A \in \mathbb{R}^{I_1 \times R}$ and $B \in \mathbb{R}^{R \times I_2 \times \dots \times I_N}$ where $Y = AB$

$$\text{rank}_{\text{Tucker-1}}(Y) = \min\{R \mid \exists A_n \in \mathbb{R}^{I_n \times R}, B \in \mathbb{R}^{R \times I_2 \times \dots \times I_N} \quad \text{s.t.} \quad Y = AB\}$$

For the Tucker and Tucker- n decompositions, we instead call a particular factorization a **rank**-(R_1, \dots, R_N) Tucker factorization or a **rank**-(R_1, \dots, R_n) Tucker- n factorization, rather than **the** CP- or Tucker-1-rank of a tensor or **the** rank of a matrix.

One reason CP and Tucker-1 only need a single rank R can be explained by considering the case when the order of the tensor $N = 2$ (matrices). The two factorizations become equivalent and are equal to low-rank R matrix factorization $Y = AB$. In fact, Tucker-1 is always equivalent to a low-rank matrix factorization, if you consider a flattening of the tensor to arrange the entries as a matrix.

The idea of tensor rank can be generalized further to constrained rank. These are the smallest rank R such that the factors in the decomposition obey the given set of constraints.

For example, the nonnegative Tucker-1 rank is defined as

$$\text{rank}_{\text{Tucker-1}}^+(Y) = \min \left\{ R \mid \exists A_n \in \mathbb{R}_+^{I_n \times R}, B \in \mathbb{R}_+^{R \times I_2 \times \dots \times I_N} \quad \text{s.t.} \quad Y = AB \right\}.$$

More restrictive constraints increase the rank of the tensor since there is less freedom in selecting the factors.

3 Computing Decompositions

- Given a data tensor and a model, how do we fit the model?

3.1 Optimization Problem

- Least squares (can use KL, 1 norm, etc.)

3.2 Base algorithm

- Use Block Coordinate Descent / Alternating Proximal Descent
 - do *not* use alternating least squares (slower for unconstrained problems, no closed form update for general constrained problems)

3.2.a Computing Gradients

- Use Auto diff generally
- But hand-crafted gradients and Lipschitz calculations *can* be faster (e.g. symmetrized slice-wise dot product)

3.2.b Computing Lipschitz Step-sizes

4 Techniques for speeding up convergences

- As stated, algorithm works
- But can be slow, especially for constrained or large problems

4.1 Sub-block Descent

- Use smaller blocks, but descent in parallel (sub-blocks don't wait for other sub-blocks)
- Can perform this efficiently with a “matrix step-size”

4.2 Momentum

- This one is standard
- Use something similar to [10]
- This is compatible with sub-block descent with appropriately defined matrix operations

4.3 Partial Projection and Rescaling

- for bounded linear constraints
 - first project
 - then rescale to enforce linear constraints
- faster to execute than a projection
- often does not lose progress because of the rescaling (decomposition dependent)

4.4 Multi-scale

- use a coarse discretization along continuous dimensions

- factorize
- linearly interpolate decomposition to warm start larger decompositions

5 Conclusion

- all-in-one package
- provide a playground to invent new decompositions
- like auto-diff for factorizations

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