Introduction to tensors in high dimensions, and their approximation

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Introduction to tensors

Let $\mathcal{A}$ be a tensor of dimension d, size $n_1 \times \cdots \times n_d$, $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \ldots n_d}$. A d-order tensor is the tensor product of d vector spaces.

- $d = 1$, first order tensors: vectors
- $d = 2$, second order tensors: matrices

Examples of solutions from problems in large dimensions in scientific computing.

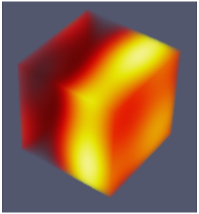

Figure: Densité de matière, projection 3d d'une densité 6d : $\int_v f(x, v)dv$

Courtesy of V. Ehrlacher and D. Lombardi

Example from scientific computing

Figure: Double stream instability for Vlasov-Poisson equation

Courtesy of V. Ehrlacher and D. Lombardi

Notations

Let $\mathcal{A}$ be a tensor of dimension d, size $n_1 \times \cdots \times n_d$, $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \ldots n_d}$.

- The element of the 3rd order tensor $\mathcal{A}$ is denoted $\mathcal{A}(i_1, i_2, i_3)$
- Fibers: defined by fixing all indices except one, e.g. for 3-order tensor: column fiber $\mathcal{A}_{:i_2 i_3}$, row fiber $\mathcal{A}_{i_1 : i_3}$, tube fiber $\mathcal{A}_{i_1 i_2 :}$
- Slices: defined by fixing all indices except two, e.g. for 3-order tensor: horizontal $\mathcal{A}_{i_1 ::}$, lateral $\mathcal{A}_{: i_2 :}$, frontal $\mathcal{A}_{:: i_3}$

Presentation using notations and following [Kolda and Bader, 2009].

Operations with tensors

- Inner product of two tensors $\mathcal{A}, \mathcal{B} \in \mathbb{R}^{n_1 \times n_2 \times \dots n_d}$ is

$$(\mathcal{A}, \mathcal{B}) = \sum_{i_1=1}^{n_1} \dots \sum_{i_d=1}^{n_d} \mathcal{A}(i_1, \dots, i_d)\mathcal{B}(i_1, \dots, i_d)$$

- The norm of $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \dots n_d}$, analogous to the Frobenius norm of a matrix, is

$$||\mathcal{A}|| = \sqrt{(\mathcal{A}, \mathcal{A})} = \sqrt{\sum_{i_1=1}^{n_1} \dots \sum_{i_d=1}^{n_d} \mathcal{A}^2(i_1, i_2, \dots, i_d)}$$

Rank-one tensors

A rank one tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \ldots n_d}$ is the outer product of d vectors,

$$\begin{aligned} \mathcal{A} &= u_1 \circ u_2 \circ \ldots \circ u_d, \text{that is} \\ \mathcal{A}(i_1, \ldots, i_d) &= u_1(i_1) \cdot \ldots \cdot u_d(i_d), \text{ for all } 1 \leq i_j \leq n_j, j = 1 \ldots d \end{aligned}$$

Unfoldings to transform a tensor into a matrix

- The mode-j unfolding of a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \dots n_d}$ represents the tensor by a matrix $A_j \in \mathbb{R}^{n_j \times N}$, where $N = n_1 \cdot \ldots \cdot n_{j-1} \cdot n_{j+1} \cdot \ldots \cdot n_d$.
- Tensor element $\mathcal{A}(i_1, \dots i_d)$ is mapped to $A(i_j, k)$, where $k = 1 + \sum_{v=1, v \neq j}^{d} (i_v - 1) N$.
- Example for $\mathcal{A} \in \mathbb{R}^{3 \times 2 \times 3}$ with the frontal slices:

$$A_{::1} = \begin{bmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{bmatrix} \; A_{::2} = \begin{bmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{bmatrix} \; A_{::3} = \begin{bmatrix} 13 & 16 \\ 14 & 17 \\ 15 & 18 \end{bmatrix}$$

The unfoldings along modes 1, 2, and 3 are:

$$A_1 = \begin{bmatrix} 1 & 4 & 7 & 10 & 13 & 16 \\ 2 & 5 & 8 & 11 & 14 & 17 \\ 3 & 6 & 9 & 12 & 15 & 18 \end{bmatrix} \; A_2 = \begin{bmatrix} 1 & 2 & 3 & 7 & 8 & 9 & 13 & 14 & 15 \\ 4 & 5 & 6 & 10 & 11 & 12 & 16 & 17 & 18 \end{bmatrix}$$

$$A_3 = \begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 7 & 8 & 9 & 10 & 11 & 12 \\ 13 & 14 & 15 & 16 & 17 & 18 \end{bmatrix}$$

Tensor multiplication along mode j with a matrix

The j-mode product of $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \ldots n_d}$ with $U \in \mathbb{R}^{K \times n_j}$ is

$$\mathcal{B} = \mathcal{A} \times_j U, \ \mathcal{B} \in \mathbb{R}^{n_1 \times \ldots \times n_{j-1} \times K \times n_{j+1} \times \ldots \times n_d},$$

$$\mathcal{B}(i_1, \ldots, i_{j-1}, k, i_{j+1}, \ldots, i_d) = \sum_{i_j=1}^{n_j} \mathcal{A}(i_1, i_2, \ldots i_d) U(k, i_j)$$

By using unfoldings, this is equivalent to:

$$B_j = U A_j$$

Some properties for j-mode matrix products:

$$\mathcal{A} \times_j U_1 \times_j U_2 = \mathcal{A} \times_j (U_2 U_1)$$
$$\mathcal{A} \times_j U_1 \times_k U_2 = \mathcal{A} \times_k U_2 \times_j U_1$$

Matrix products

- The Kronecker product of $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{k \times j}$ is $C \in \mathbb{R}^{(mk)\times(nj)}$,

$$C = A \otimes B = \begin{bmatrix} A(1,1)B & \dots & A(1,n)B \\ \vdots & \ddots & \vdots \\ A(m,1)B & \dots & A(m,n)B \end{bmatrix}$$

- The Khatri-Rao product of two matrices $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{k \times n}$ is $C \in \mathbb{R}^{(mk)\times n}$

$$C = A \odot B = [A(:,1) \otimes B(:,1) \dots A(:,n) \otimes B(:,n)]$$

- The Hadamard product of two matrices $A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{m \times n}$ is $C \in \mathbb{R}^{m \times n}$, computed as the elementwise matrix product:

$$C = A * B = \begin{bmatrix} A(1,1)B(1,1) & \dots & A(1,n)B(1,n) \\ \vdots & \ddots & \vdots \\ A(n,1)B(n,1) & \dots & A(n,n)B(n,n) \end{bmatrix}$$

Some properties of matrix products

$$
\begin{aligned}
(A \odot B)^T (A \odot B) &= A^T A * B^T B, \\
(A \odot B)^+ &= ((A^T A) * (B^T B))^+ (A \odot B)^T
\end{aligned}
$$

where A^+ denotes the Moore-Penrose pseudoinverse of A.
Given a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \ldots n_d}$ and matrices $U_i \in \mathbb{R}^{m \times n_i}$ for all $1 \leq i \leq d$

$$
\begin{aligned}
\mathcal{B} &= \mathcal{A} \times_1 U_1 \times_2 U_2 \ldots \times_d U_d \\
&\Leftrightarrow \quad B_i = U_i A_i (U_d \otimes \ldots \otimes U_{i+1} \otimes U_{i-1} \otimes \ldots \otimes U_1)^T
\end{aligned}
$$

Rank of a tensor

The rank of a tensor is the number of terms in the CP decomposition that computes exactly the tensor, that is $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \dots n_d}$ has rank k if

$$\mathcal{A} = \sum_{i=1}^{k} u_i^1 \circ u_i^2 \circ \ldots \circ u_i^d$$

where $u_i^1 \circ u_i^2$ is the outer product of u_i^1 and u_i^2.

- Determining the rank of a tensor is an NP-problem in general [Hastad, 1990]
- Given a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$, its maximum rank is bounded as:

$$rank(\mathcal{A}) \leq \min(n_1 n_2, n_1 n_3, n_2 n_3)$$

- If the vectors a_i^1 form the columns of a matrix A^1, respectively the vectors a_i^2 and a_i^3 form A^2, A^3 and $rank(A^i) = k_i$, then the above decomposition is unique [Kruskal, 1989, Kruskal, 1977] if

$$k_1 + k_2 + k_3 \geq 2k + 2$$

Plan

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Low rank approximation algorithms

Main low rank approximation algorithms

- CANDECOMP/PARAFAC (CP): tensor decomposed as a sum of rank-one tensors: proposed by Hitchcock in 1927.
- Tucker decomposition: introduced by Tucker in 1963 [Tucker, 1963], can be computed by using high order SVD (HOSVD)
- Tensor train for high dimensions

CP decomposition

Computes an approximation by factoring a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \dots n_d}$ into the sum of k rank-one tensors.

$$\mathcal{A} \approx \sum_{i=1}^{k} u_{1,i} \circ u_{2,i} \circ \dots \circ u_{d,i}$$

If k is given, then the CP is typically computed by the Alternating Least Squares (ALS) algorithm, that is solve

$$\min_{\mathcal{A}'} ||\mathcal{A} - \mathcal{A}'|| \text{ with } \mathcal{A}' = \sum_{i=1}^{k} \alpha_k u_{1,i} \circ u_{2,i} \circ \dots \circ u_{d,i}$$

- Let matrix $U_j \in \mathbb{R}^{n_j \times k}$ be formed by vectors $u_{j,i}$, $i = 1, \dots, k$, for all $j = 1, \dots, d$.

CP decomposition (contd)

- Let matrix $U_j \in \mathbb{R}^{n_j \times k}$ be formed by vectors $u_{j,i}$, $i = 1, \ldots, k$, for all $j = 1, \ldots, d$.

If $\mathcal{A}' = \sum_{i=1}^{k} \alpha_k u_{1,i} \circ u_{2,i} \circ \ldots \circ u_{d,i}$,
we can write in matricized form

$$\begin{aligned} {A'}_1 &= U_1(U_3 \odot U_2)^T \\ {A'}_2 &= U_2(U_3 \odot U_1)^T \\ {A'}_3 &= U_3(U_2 \odot U_1)^T \end{aligned}$$

CP decomposition (contd)

- ALS fixes $U_2, \ldots, U_d$ and minimizes for U_1, then fixes $U_1, U_3, \ldots U_d$ and minimizes for U_2, and so on until some error criterion is met.
- For $U_2, \ldots, U_d$ fixed, ALS minimizes:

$$\min_{U_1'} ||A_1 - U_1'(U_3 \odot U_2)^T||_F$$

- The optimal solution is

$$U_1' = A_1(U_3 \odot U_2)^{+T} = A_1(U_3 \odot U_2)(U_3^T U_3 * U_2^T U_2)$$

where U^+ denotes the Moore-Penrose pseudoinverse of U.
- U_i can be chosen to be random or equal to leading left singular vectors of A_i, for all $1 \leq i \leq d$.

ALS for computing a CP decomposition

Algorithm 1 ALS for computing a *rank* $-$ *k* approximation

Input: Tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$, rank k

Initialize $U_i \in \mathcal{R}^{n_i \times k}$ for all $1 \leq i \leq d$

repeat

    for $i = 1$ to d **do**

        $V = U_1^T U_1 * \dots * U_{i-1}^T U_{i-1} * U_{i+1}^T U_{i+1} * \dots U_d^T U_d$, where $V \in \mathbb{R}^{k \times k}$

        $U_i = A_i (U_d \odot \dots \odot U_{i+1} \odot U_{i-1} \odot \dots \odot U_1) V^+$

        Normalize columns of U_i, store result in α

    end for

until maximum iterations reached or no further improvement obtained

Return: α, $U_1, U_2, \dots, U_d$

d-rank of a tensor

Given tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \ldots \times n_d}$, if for every unfolding A_i we have $k_i = rank(A_i)$, then we say $\mathcal{A}$ is a $rank - (k_1, \ldots, k_d)$ tensor.

Tucker decomposition

- Compute an approximation $\mathcal{A}'$ by decomposing a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \ldots \times n_d}$ into the product of a core tensor $\mathcal{C}$ and matrices $U_i, i = 1, \ldots, d$.

$$\begin{aligned} \mathcal{A}' &= \mathcal{C} \times_1 U_1 \times_2 U_2 \ldots \times_d U_d \\ &= \sum_{s_1=1}^{k_1} \sum_{s_2=1}^{k_2} \ldots \sum_{s_d=1}^{k_d} \mathcal{C}(s_1, \ldots, s_d) U_1(:, s_1) \circ \ldots \circ U_d(:, s_d) \end{aligned}$$

  where $\mathcal{C} \in \mathbb{R}^{k_1 \times k_2 \times \ldots \times k_d}$, $U_i \in \mathbb{R}^{n_i \times k_i}$, $i = 1, \ldots d$.
- The matrices $U_i, i = 1, \ldots, d$ are usually orthogonal and are (or approximate) the left singular vectors of A_i, the unfolding along mode i.
- The formula to compute the value of a Tucker tensor at a given point, for $i_j = 1, \ldots n_j$ and $1 \leq j \leq d$ is:

$$\mathcal{A}(i_1, ..., i_d) = \sum_{1 \leq s_j \leq k_j, 1 \leq j \leq d} \mathcal{C}(s_1, ..., s_d) U_1(i_1, s_1) \cdots U_d(i_d, s_d)$$

HOSVD for computing a Tucker decomposition

Algorithm 2 HOSVD (High Order SVD) for computing a $rank-(k_1, k_2, \ldots k_d)$ approximation

Input: Tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, ranks $k_1, \ldots k_d$

1: **for** $i = 1$ to d **do**

2: For every unfolding A_i along mode i compute the k_i truncated SVD of A_i, $A_i = U_i \Sigma_i V_i^T$, where $U_i \in \mathbb{R}^{n_i \times k_i}$

3: **end for**

4: $\mathcal{C} = \mathcal{A} \times_1 U_1^T \times_2 U_2^T \ldots \times_d U_d^T$

Return: $\mathcal{C}$, $U_1, U_2, \ldots, U_d$

It can be used as a starting point for ALS algorithm.

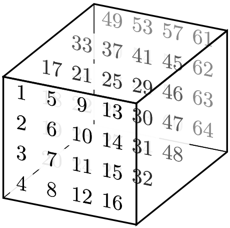
HOSVD for computing a Tucker decomposition

HOSVD for computing a $rank - (k_1, \dots k_d)$ approximation

1. **Input**: Tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$, ranks $k_1, \dots k_d$
2. For every unfolding A_i along mode $i = 1...d$ compute the k_i (approximated) leading left singular vectors of A_i, $Q_i \in \mathbb{R}^{n_i \times k_i}$

$$A_1 = \begin{bmatrix} 1 & 5 & 9 & 13 & 17 & 21 & 25 & 29 & 33 & 37 & 41 & 45 & 49 & 53 & 57 & 61 \\ 2 & 6 & 10 & 14 & 18 & 22 & 26 & 30 & 34 & 38 & 42 & 46 & 50 & 54 & 58 & 62 \\ 3 & 7 & 11 & 15 & 19 & 23 & 27 & 31 & 35 & 39 & 43 & 47 & 51 & 55 & 59 & 63 \\ 4 & 8 & 12 & 16 & 20 & 24 & 28 & 32 & 36 & 40 & 44 & 48 & 52 & 56 & 60 & 64 \end{bmatrix} \rightarrow RRQR \begin{bmatrix} 61 & 1 \\ 62 & 2 \\ 63 & 3 \\ 64 & 4 \end{bmatrix}$$

3. $\mathcal{C} = \mathcal{A} \times_1 Q_1^T \times_2 Q_2^T \dots \times_d Q_d^T$
4. **Return:** $\mathcal{A}' = \mathcal{C} \times_1 Q_1 \dots \times_d Q_d = \mathcal{A} \times_1 Q_1 Q_1^T \dots \times_d Q_d Q_d^T$



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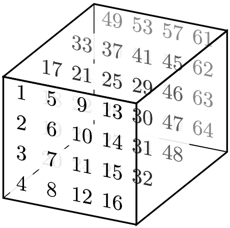

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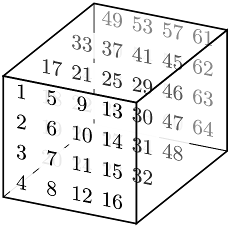

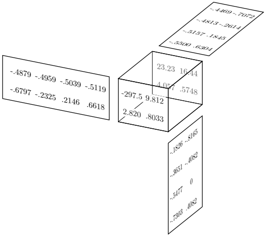

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Error bound:

If Q_i are the leading left singular vectors of unfolding A_i, then:

$$\|\mathcal{A} - \mathcal{A}'\|_F \leq \sqrt{d} \|\mathcal{A} - \mathcal{A}_{best}\|_F,$$

where $\mathcal{A}_{best}$ is the best rank-$k_1, \dots, k_d$ approximation of $\mathcal{A}$.

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