250085 VU
TENSOR METHODS FOR DATA SCIENCE AND SCIENTIFIC COMPUTING
WINTER SEMESTER 2021

HOMEWORK ASSIGNMENT 5

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Due by **11:30 on Thursday, 16th December 2021**. To be submitted via Moodle.

The theoretical part may be (i) typeset, (ii) handwritten digitally or (iii) handwritten on a physical medium and then digitized by scanning or photographing. For the programming part, any programming language and environment may be used.

For each student submitting a solution, the submission should consist of (i) a single PDF file presenting the solution of the theoretical part and the results of the programming part in a self-contained fashion (so that running the student's code not be required for understanding the results) and (ii) the code (if any), ready to run and reproduce the results presented in the PDF file, organized in any reasonable number of files.

1. Implementing the MPS-TT truncation.

Implement the MPS-TT rounding (rank truncation) algorithm. Given (i) a vector $\boldsymbol{u} \in \mathbb{R}^{n_1 \cdots n_d}$ (where $d \in \mathbb{N}$ and $n_1, \ldots, n_d \in \mathbb{N}$) in the form of an MPS-TT factorization $\boldsymbol{u} = U_1 \bowtie \cdots \bowtie U_d$ with ranks $p_1, \ldots, p_{d-1} \in \mathbb{N}$ and (ii) target ranks $r_1, \ldots, r_{d-1} \in \mathbb{N}$, the implementation should produce an MPS-TT approximation $\boldsymbol{v} = V_1 \bowtie \cdots \bowtie V_d$ to $\boldsymbol{u}$ of quasi-optimal accuracy in the Frobenius norm and of ranks not exceeding $r_1, \ldots, r_{d-1}$.

The output should include (i) the MPS-TT decomposition produced by the algorithm, (ii) the vectors of singular values of the matrices that are explicitly approximated within the algorithm (one vector of singular values per step) and (iii) the Frobenius norms of the errors of the mentioned low-rank matrix approximation (one scalar per step).

2. Adding, scaling and multiplying in the TT-MPS representation.

Implement functions that, for $d \in \mathbb{N}$ and $m_1, \ldots, m_d, n_1, \ldots, n_d \in \mathbb{N}$, compute exact MPS-TT factorizations $\boldsymbol{w} = W_1 \bowtie \cdots \bowtie W_d$

a) of the linear combination $\boldsymbol{w} = \alpha \boldsymbol{u} + \beta \boldsymbol{v} \in \mathbb{R}^{n_1 \cdots n_d}$, with given coefficients $\alpha, \beta \in \mathbb{R}$, of two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^{n_1 \cdots n_d}$ given in the form of MPS-TT decompositions $\boldsymbol{u} = U_1 \bowtie \cdots \bowtie U_d$ and $\boldsymbol{v} = V_1 \bowtie \cdots \bowtie V_d$;

b) of the entrywise product $\boldsymbol{w} = \boldsymbol{u} \odot \boldsymbol{v} \in \mathbb{R}^{n_1 \cdots n_d}$, of two vectors $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{R}^{n_1 \cdots n_d}$ given in the form of MPS-TT decompositions $\boldsymbol{u} = U_1 \bowtie \cdots \bowtie U_d$ and $\boldsymbol{v} = V_1 \bowtie \cdots \bowtie V_d$;

c) of the product $\boldsymbol{w} = \boldsymbol{A}\boldsymbol{u} \in \mathbb{R}^{m_1 \cdots m_d}$ of a given matrix $\boldsymbol{A} \in \mathbb{R}^{m_1 \cdots m_d \times n_1 \cdots n_d}$ and a given vector $\boldsymbol{u} \in \mathbb{R}^{n_1 \cdots n_d}$ given in the form of MPS-TT decompositions $\boldsymbol{A} = A_1 \bowtie \cdots \bowtie A_d$ and $\boldsymbol{u} = U_1 \bowtie \cdots \bowtie U_d$.

3. Testing the MPS-TT arithmetic. For $n = 51$, let us consider the grid of

$$t_i = 2\,\frac{i-1}{n-1} - 1 \quad \text{with} \quad i = 1, \ldots, n\,,$$

the tensors $\boldsymbol{X}, \boldsymbol{Y} \in \mathbb{R}^{n \times n \times n \times n}$ given by

$$x_{i_1,\ldots,i_4} = T_p\left(\sum_{k=1}^{4} \frac{t_{i_k}}{k}\right) \quad \text{and} \quad y_{i_1,\ldots,i_4} = T_q\left(\sum_{k=1}^{4} \frac{t_{i_k}}{k}\right),$$

where $p, q \in \mathbb{N}_0$ and T_r with $r \in \mathbb{N}_0$ is the Chebyshev polynomials of the first kind of degree r, and their vectorizations

$$\boldsymbol{x} = \operatorname{vec} \boldsymbol{X} \quad \text{and} \quad \boldsymbol{y} = \operatorname{vec} \boldsymbol{Y}\,.$$

Consider the sum $\boldsymbol{s} = \boldsymbol{x} + \boldsymbol{y}$ and the entrywise product $\boldsymbol{z} = \boldsymbol{x} \odot \boldsymbol{y}$.

a) Inspect the decay of the singular values for all the MPS-TT unfoldings of $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{s}, \boldsymbol{z}$ for several moderate values of p and q (for example, 3 and 4, 5 and 7) For each of these vectors, how does the maximum of the MPS-TT ranks depend on p and q? Are the bounds derived for such vectors in the lectures sharp for the examples you have considered?

b) Let $p = 5$ and $q = 7$. Compute exact (up to machine precision) MPS-TT representations of $\boldsymbol{x}$ and $\boldsymbol{y}$ using an implementation of the TT-SVD (Schmidt decomposition) algorithm (see Assignment 4). Use your implementation from Problem **2.** to directly assemble MPS-TT representations of $\boldsymbol{s}$ and $\boldsymbol{z}$ without forming these vectors entrywise. Use your implementation of the rank truncation algorithm from Problem **1.** to compute exact (up to machine precision) MPS-TT representations of $\boldsymbol{s}$ and $\boldsymbol{z}$. Check that these decompositions are exact up to machine precision by forming the vectors entrywise (as $\boldsymbol{x} + \boldsymbol{y}$ and $\boldsymbol{x} \odot \boldsymbol{y}$).