University of Vienna
Faculty of Mathematics

TENSOR METHODS FOR DATA SCIENCE AND SCIENTIFIC COMPUTING

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December 15, 2021

Contents

1 Assignment 5

1.1 Truncated TT-MPS

Given an MPS-TT factorization $U_1,\dots,U_d$ of $A \in \mathbb{R}^{n_1\times\cdots\times n_d}$, with ranks $p_1,\dots,p_{d-1} \in \mathbb{N}$, we will produce a MPS-TT approximation of ranks not exceeding $r_1,\dots,r_{d-1}$ with factors $V_1,\dots,V_d$ of quasioptimal accuracy in the Forbenius norm.

Algorithm 1 rank truncation MPS-TT

$\tilde{U}_1 \leftarrow U_1$
for $k = 1,\dots,d-1$ **do**
  $\tilde{U}_k \leftarrow \text{reshape}\left(\tilde{U}_k,(p_{k-1}\cdot n_k, r_k\right)$
  $\bar{U}_k \leftarrow \hat{P}_k\hat{\Sigma}_k\hat{W}_k^*$ ▷ rank- r_k T-SVD of $\tilde{U}_k$
  $\hat{Q}_k \leftarrow \text{reshape}\left(\hat{P}_k,(p_{k-1},n_k,r_k)\right)$
  $\hat{Z}_k \leftarrow \text{reshape}\left(\hat{\Sigma}_k\hat{W}_k^*,(r_k,1,p_k)\right)$
  $(\tilde{U}_{k+1})_{\beta_k,i_{k+1},\alpha_{k+1}} \leftarrow \sum_{\alpha_k=1}^{r_k}(\hat{Z}_k)_{\beta_k,1,\alpha_k}(U_{k+1})_{\alpha_k,i_{k+1},\alpha_{k+1}}$
  save$(\hat{Q}_k)$
end for
save $\left(\tilde{U}_d\right)$

1.2 TT-MPS arithmetic

1.2.1 Addition

Consider two tensors U and V of size $n_1\times\cdots\times n_d \in \mathbb{N}$ for $d\in\mathbb{N}$, with TT-MPS factorization U_k with rank p_k and V_k with rank q_k respectively (for $k\in\{1,\dots,d-1\}$). Then TT-MPS factorization of $W = U+V$ can be calculated without evaluating U or V, just by using $U_1,\dots,U_d$ and $V_1,\dots,V_d$ by the following

$$\begin{aligned}W &= U_1 \bowtie \cdots \bowtie U_d + V_1 \bowtie \cdots \bowtie V_d = \\ &= \begin{bmatrix} U_1 & V_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 \bowtie \cdots \bowtie U_d \\ V_2 \bowtie \cdots \bowtie V_d \end{bmatrix} = \\ &= \cdots = \\ &= \begin{bmatrix} U_1 & V_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & 0 \\ 0 & V_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} U_{d-1} & 0 \\ 0 & V_{d-1} \end{bmatrix} \bowtie \begin{bmatrix} U_d \\ V_d \end{bmatrix} = \\ &= W_1 \bowtie \cdots \bowtie W_d, \end{aligned} \tag{1}$$

where W has a decomposition of ranks $(p_1+q_1),\dots,(p_{d-1}q_{d-1})$. The construction of these matrices and vectors can be done by initializing the W_k and then slicing for U_k and V_k in the second dimension, meaning n_k. Thereby for the k-th ($2 \le k \le d-2$) step we would have

$$(W_k)_{:,i_k,:} = \begin{bmatrix} (U_k)_{:,i_k,:} & 0 \\ 0 & (V_k)_{:,i_k,:} \end{bmatrix} \quad \forall i_k \in \{1,\dots,n_k\}. \tag{2}$$

For the first step we have $p_0 = q_0 = 1$ and thereby

$$(W_1)_{:,i_1,:} = \begin{bmatrix} (U_1)_{1,i_1,:} & (V_1)_{1,i_1,:} \end{bmatrix} \quad \forall i_1 \in \{1,\dots,n_1\}. \tag{3}$$

And for the $k = d$-th step we have $p_d = q_d = 1$ and thereby

$$(W_d)_{:,i_d,:} = \begin{bmatrix} (U_d)_{:,i_d,1} \\ (V_d)_{:,i_d,1} \end{bmatrix} \quad \forall i_d \in \{1,\dots,n_d\}. \tag{4}$$

This concludes the construction of the algorithm for addition

1.2.2 Hadamard Product

Now consider again two tensors U and V of size $n_1 \times \cdots \times n_d \in \mathbb{N}$ for $d \in \mathbb{N}$, with TT-MPS factorization U_k with rank p_k and V_k with rank q_k respectively (for $k \in \{1,\dots,d-1\}$). Then TT-MPS factorization of $W = U \otimes V$ can be calculated without evaluating U or V, just by using $U_1,\dots,U_d$ and $V_1,\dots,V_d$ by the following

$$\begin{aligned} W_{i_1,\dots,i_d} &= \sum_{\alpha_1=1}^{q_1} \cdots \sum_{\alpha_{d-1}=1}^{q_{d-1}} \prod_{k=1}^{d} U_k(\alpha_{k-1}, i_k, \alpha_k) \cdot \sum_{\beta_1=1}^{q_1} \cdots \sum_{\beta_{d-1}=1}^{q_{d-1}} \prod_{k=1}^{d} V_k(\beta_{k-1}, i_k, \beta_k) = \\ &= \sum_{\gamma_1=1}^{r_1} \cdots \sum_{\gamma_{d-1}=1}^{r_{d-1}} \prod_{k=1}^{d} W_k(\gamma_{k-1}, i_k, \gamma_k). \end{aligned} \tag{5}$$

Thereby the factors W_k can be calculated with the factor wise product

$$W_k(\alpha_{k-1}\beta k - 1, i_k, \alpha_k\beta_k) = U_k(\alpha_{k-1}, i_k, \alpha_k) \cdot V_k(\beta_{k-1}, i_k, \beta_k), \tag{6}$$

for all $\alpha_k \in \{1,\dots,p_k\}$ and $\beta_k \in \{1,\dots,q_k\}$ and $p_0 = p_d = q_0 = q_d = 1$. Where the TT-MPS calculated by the algorithm is of ranks $(p_1q_1),\dots,(p_{d-1}q_{d-1})$.

The computer reads in slices and Kronecker products

$$(W_k)_{:,i_k,:} = (U_k)_{:,i_k,:} \otimes (V_k)_{:,i_k,:} \quad \forall i_k \in \{1,\dots,n_k\}. \tag{7}$$

1.2.3 Matrix Vector product

Now consider $A \in \mathbb{R}^{n_1\cdots n_d \times m_1\cdots m_d}$ and $u \in \mathbb{R}^{m_1\cdots m_d}$. The TT-MPS factorization of A is $A_k \in \mathbb{R}^{p_{k-1}\times n_k \times m_k \times q_k}$ and the TT-MPS factorization of U is $U_k \in \mathbb{R}^{q_{k-1}\times m_k \times q_k}$. The TT-MPS factors W_k of $w = A \cdots u$ can be explicitly calculated with

$$
\begin{aligned}
W_{i_1,\dots,i_d} &= \sum_{j_1,\dots,j_d} A_{i_1\cdots i_d, j_1\cdots j_d} U_{j_1\cdots j_d} \\
&= \sum_{j_1,\dots,j_d} \sum_{\alpha_1=1}^{p_1} \cdots \sum_{\alpha_{d-1}=1}^{p_{d-1}} \prod_{k=1}^{d} A_k(\alpha_{k-1}, i_k, j_k, \alpha_k) \cdot \sum_{\beta_1=1}^{q_1} \cdots \sum_{\beta_{d-1}=1}^{q_{d-1}} \prod_{k=1}^{d} U_k(\beta_{k-1} j_k, \beta_k) \cdot \\
&= \sum_{\alpha_1\beta_1} \cdots \sum_{\alpha_{d-1}\beta_{d-1}} \prod_{k=1}^{d} \left(\sum_{j_k}^{n_k} A_k(\alpha_{k-1}, i_k, j_k, \alpha_k) U_K(\beta_{k-1}, j_k, \beta_k) \right) \\
&= \sum_{\gamma_1}^{r_1} \cdots \sum_{\gamma_{d-1}}^{r_{d-1}} \prod_{k=1}^{d} W_k(\gamma_{k-1}, i_k, \gamma_k),
\end{aligned} \tag{8}
$$

for $r_k = q_k \cdot p_k$. The computer reads

$$
(W_k)_{:,i_k,:} = \sum_{j_k=1}^{n_k} (A_k)_{:,i_k,j_k,:} \otimes (U_k)_{:,j_k,:} \quad \forall i_k \in \{1,\dots,n_k\} \tag{9}
$$

for all $k = 1,\dots,d$

1.3 Testing

Consider the grid for $n = 51$

$$
t_i = 2\frac{i-1}{n-1} - 1 \quad i = 1,\dots,n \tag{10}
$$

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

$$
x_{i_1,\dots,i_4} = T_p\left(\sum_{k=1}^{4} \frac{t_{i_k}}{4}\right) \tag{11}
$$

$$
y_{i_1,\dots,i_4} = T_q\left(\sum_{k=1}^{4} \frac{t_{i_k}}{4}\right) \tag{12}
$$

$$
\tag{13}
$$

for $p, q \in \mathbb{N}_0$ and T_r is the Chebyshev polynomial for a $k \in \mathbb{N}_0$. The Chebyshev polynomials are defined by

$$
T_r(x) = \begin{cases} \cos(r\cdot\arccos(x)) & |x| \le 1 \\ \cosh(r\cdot\operatorname{arccosh}(x)) & x \ge 1 \\ (-1)^r \cosh(r\cdot\operatorname{arccosh}(x)) & x \le -1 \end{cases} . \tag{14}
$$

Additionally we define

$$
S := X + Y \tag{15}
$$

$$
Z := X \otimes Y. \tag{16}
$$

The following figures show for $(p,q) = 3,4$ and $(p,q) = 5,7$ the TT-MPS unfolding singular values of tensors X, Y, S, Z.

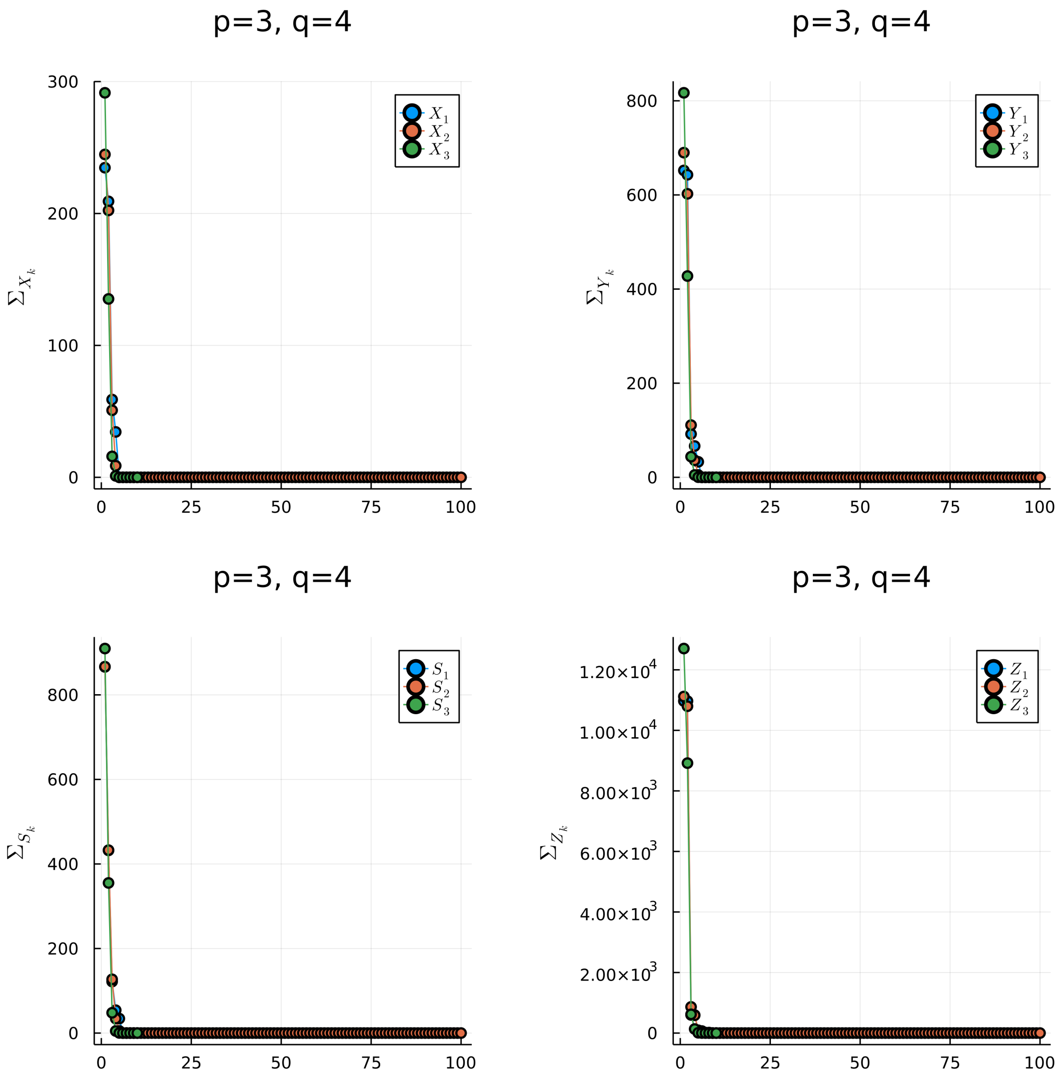

Figure 1: Some text

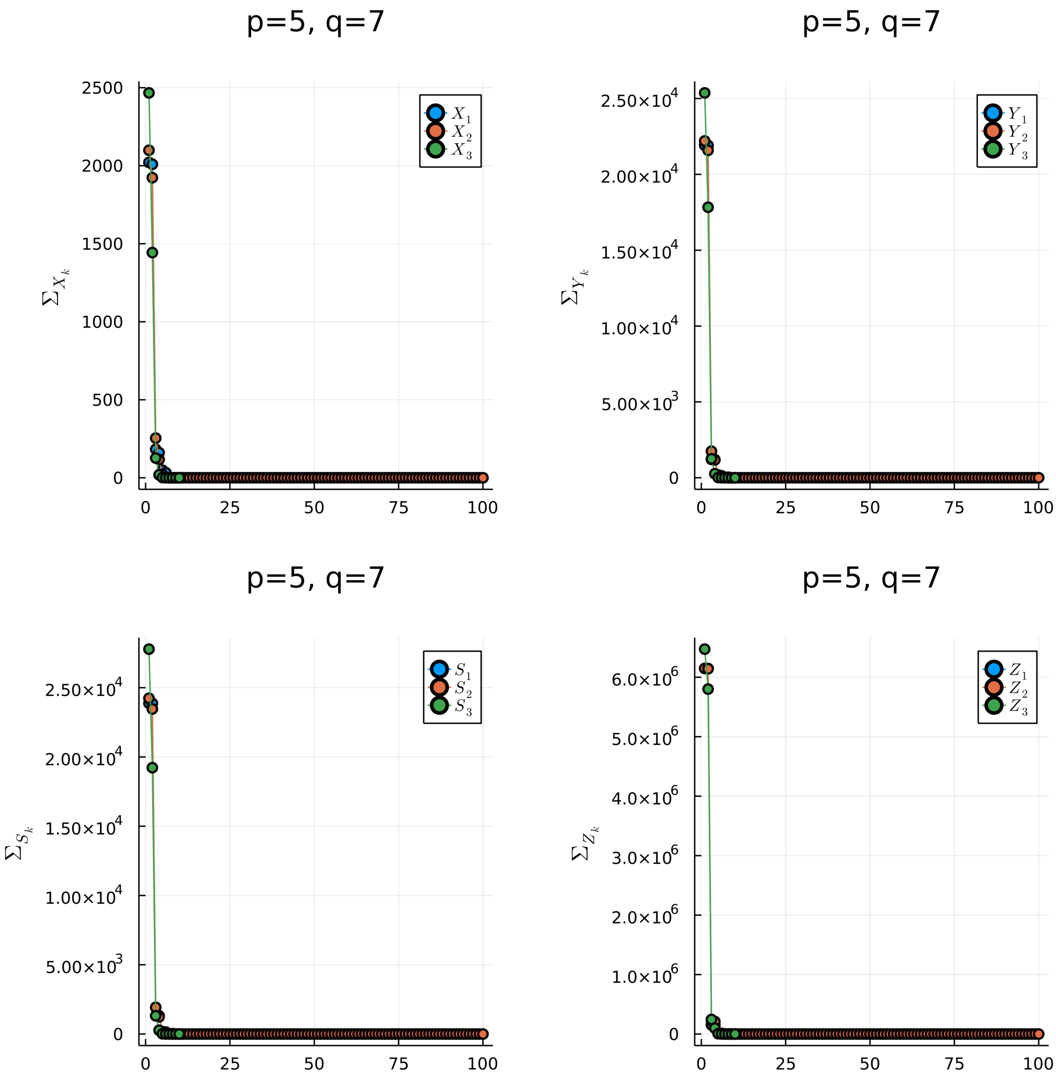

Figure 2: Some text

The following figures show the ranks MPS-TT unfolding matrices of X,Y,S,Z for $(p,q) = 3,4$ and $(p,q) = 5,7$ respectively

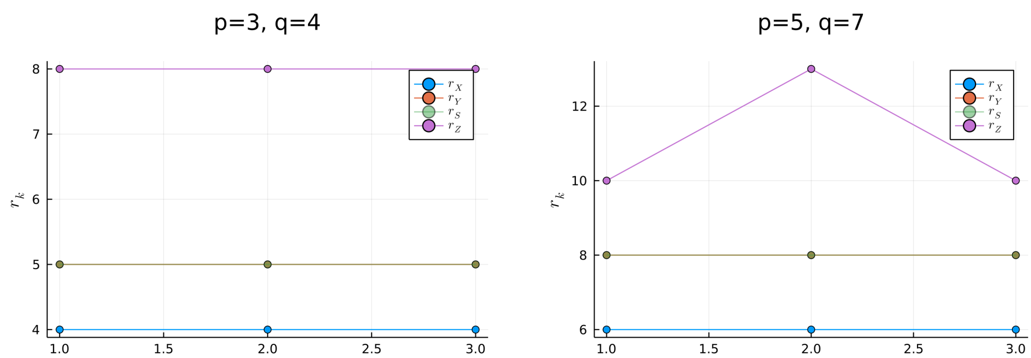

Figure 3: Some text

References

[1] Popovic Milutin. *Git Instance, Tensor Methods for Data Science and Scientific Computing*. URL: git://popovic.xyz/tensor_methods.git.