Homework 12

Tensor Train Singular Value Decomposition (TTSVD)

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Problem 1. We will go to implement the TT-SVD (Tensor Train Singular Value Decomposition) algorithm. The TT Decomposition of a N-order tensor $\mathcal{X} \in \mathbb{R}^{I_1 \times I_2 \times \cdots \times I_N}$, with TT-Ranks $(R_1, R_2, \cdots, R_{N-1})$, is a decomposition of the tensor \mathcal{X} into a train of tensors as

$$\mathcal{X} = \mathbf{G}_1 \times_2^1 \mathcal{G}_2 \times_3^1 \mathcal{G}_3 \times_4^1 \cdots \times_{N-1}^1 \mathcal{G}_{N-1} \times_N^1 \mathbf{G}_N.$$

For a 4-order tensor $\mathcal{X} \in \mathbb{R}^{5 \times 5 \times 5 \times 5}$, implement the TT-SVD algorithm to estimate the TT-cores $\mathbf{G}_1 \in \mathbb{C}^{5 \times R_1}$, $\mathcal{G}_2 \in \mathbb{C}^{R_1 \times 5 \times R_2}$, $\mathcal{G}_3 \in \mathbb{C}^{R_2 \times 5 \times R_3}$, and $\mathbf{G}_4 \in \mathbb{C}^{R_3 \times 5}$ that forms the TT Decomposition of \mathcal{X} , for given ranks (R_1, R_2, R_3) . For randomly generated $(\mathbf{G}_1, \mathcal{G}_2, \mathcal{G}_3, \mathbf{G}_4)$, compare the original tensor \mathcal{X} with the one reconstructed by the TT-SVD.

Solution.

The function is implemented in Julia (v1.4), and is shown in Listing 1. Regarding the present implementation, lines 2–14 define an auxiliary function to compute the tensor train products. The Train Tensor Singular Value Decomposition (TT-SVD) algorithm is then implemented in lines 17–237, following the pseudocode provided in the course material.

```
# ==== FUNCTIONS ====
 1
      # The Tensor-Train product function
 2
      function ×¹(G...)
 3
            # Auxiliary variables with dimension/rank information
 4
            IR = [size(G[1]); [size(G[i])[2:end] for i=2:length(G)]...]
 5
            I,R = ([IR[i][1] \text{ for } i=1:length(G)], [IR[i][2] \text{ for } i=1:length(G)-1])
 6
 7
 8
            # Tensor-train product loop
            \mathcal{X} = zeros(I...)
 9
            for i in CartesianIndices(\mathcal{X}), r in CartesianIndices((\mathbb{R}[1],\mathbb{R}[2],\mathbb{R}[3]))
10
                  \mathcal{X}[i] += G[1][i[1],r[1]]*G[2][r[1],i[2],r[2]]*G[3][r[2],i[3],r[3]]*G[4][r[3],i[4]]
11
12
            return \mathcal{X}
                              # Returns the resulting tensor
13
14
15
      # The Tensor-Train Singular Value Decomposition (TTSVD) algorithm
16
      function TTSVD(\mathcal{X})
17
            I = size(\mathcal{X})
                                                                                    # Auxiliary variable
18
19
            X^1 = \text{reshape}(\mathcal{X}, (I[1], \Pi(I[2:4])))
                                                                                    # Unfolds the tensor [\mathcal{X}]_1 \in \mathbb{R}(I_1,I_2I_3I_4)
20
                                                                                    # Computes the SVD [\mathcal{X}]_1 = \mathbf{U} \Sigma \mathbf{V}^H
            U, \Sigma, V = svd(X^1);
                                        \Sigma = Diagonal(\Sigma);
21
            R_1 = sum(diag(\Sigma) .> 1e-6)
                                                                                   # Gets the number of nonzero singular-values
22
            U_1 = U[:,1:R_1]; V_1 = (\Sigma * (V)^H)[1:R_1,:]
                                                                                   # Truncates pair (U,V) given R<sub>1</sub>
23
                                                                                  # Stores the 1st factor \mathtt{G}_1 \in \mathbb{R}(\mathtt{I}_1,\mathtt{R}_1)
            G_1 = U_1
24
25
                                                                                   # Unfolds the matrix \mathtt{X^2} = [\mathtt{V}_1]_1 \in \mathbb{R}(\mathtt{R}_1\mathtt{I}_2,\mathtt{I}_3\mathtt{I}_4)
            X^2 = \text{reshape}(V_1, (R_1*I[2], \Pi(I[3:4])))
26
            U, \Sigma, V = svd(X^2);
                                       \Sigma = Diagonal(\Sigma);
                                                                                    # Computes the SVD X^2 = U \Sigma V^H
27
                                                                                   # Gets the number of nonzero singular-values
            R_2 = sum(diag(\Sigma) .> 1e-6)
28
            \mathbf{U}_{2} = \mathbf{U}[:,1:\mathbf{R}_{2}]; \quad \mathbf{V}_{2} = (\Sigma * (\mathbf{V})^{H})[1:\mathbf{R}_{2},:]
\mathcal{G}_{2} = \text{reshape}(\mathbf{U}_{2}, (\mathbf{R}_{1}, \mathbf{I}[2], \mathbf{R}_{2}))
                                                                                   # Truncates pair (U,V) given R_2
29
                                                                                  # Reshapes the 2nd factor \mathcal{G}_2 \in \mathbb{R}(\mathtt{R}_1,\mathtt{I}_2,\mathtt{R}_2)
30
31
            X^3 = \text{reshape}(V_2, (R_2*I[3], I[4]))
                                                                                  # Unfolds the matrix X^3 = [V_2]_1 \in \mathbb{R}(R_2I_3, I_4)
32
            U, \Sigma, V = svd(X^3); \qquad \Sigma = Diagonal(\Sigma);
                                                                                    # Computes the SVD X^3 = U \Sigma V^H
33
            R_3 = sum(diag(\Sigma) .> 1e-6)
                                                                                   # Gets the number of nonzero singular-values
34
            U_3 = U[:,1:R_3]; V_3 = (\Sigma * (V)^H)[1:R_3,:]
                                                                                   # Truncates pair (U,V) given R3
35
            \mathcal{G}_3 = reshape(U<sub>3</sub>, (R<sub>2</sub>, I[3], R<sub>3</sub>))
                                                                                  # Reshapes the 3rd factor \mathcal{G}_3 \in \mathbb{R}(\mathtt{R}_2,\mathtt{I}_3,\mathtt{R}_3)
36
            G_4 = V_3[1:R_3,:]
                                                                                  # Stores the 4th factor G_4 \in \mathbb{R}(R_3, I_4)
37
38
            return (G_1, G_2, G_3, G_4)
                                                                                  # Returns the decomposition factors
39
40
      end
```

Listing 1: The Tensor-Train Singular Value Decomposition (TTSVD) algorithm for Problem 1.

The function $\times^1(\cdot)$ implements the element-wise TT decomposition through the formula

$$x_{i_1,i_2,\cdots,i_N} = \sum_{r_1=1}^{R_1} \sum_{r_2=1}^{R_2} \sum_{r_3=1}^{R_3} \cdots \sum_{r_{N-2}=1}^{R_{N-2}} \sum_{r_{N-1}=1}^{R_{N-1}} \mathbf{G}_{1_{i_1,r_1}} \mathcal{G}_{2_{r_1,i_2,r_2}} \mathcal{G}_{3_{r_2,i_3,r_3}} \cdots \mathcal{G}_{N-1_{r_{N-2},i_{N-1},r_{N-1}}} \mathbf{G}_{N_{r_N,i_{N-1}}}.$$

The TT-SVD algorithm follows the procedure described by the tensor network shown in Fig. 1

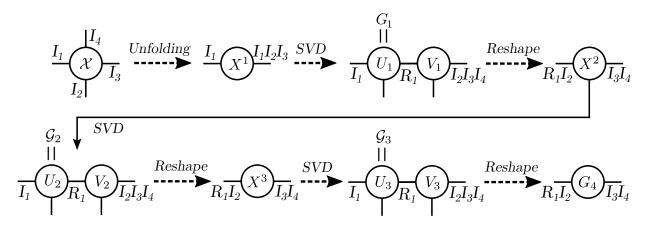


Figure 1: Illustration of the TT-SVD algorithm using a Tensor Network framework.

The implementation is tested through the script presented at Listing 2. The execution of the assertion tests at lines 10 and 18 do not result in any failed assertion, thus indicating that the function outputs the expected results for the given tests. Specifically, executing lines 11 and 19 shows that, on average, $\|\mathcal{X} - \hat{\mathcal{X}}\|_F^2 \approx 1.2 \cdot 10^{-26}$ for $\hat{\mathcal{X}} = \hat{\mathbf{G}}_1 \times_2^1 \hat{\mathcal{G}}_2 \times_3^1 \hat{\mathcal{G}}_3 \times_4^1 \hat{\mathbf{G}}_4$ with all TT-cores obtained from the TT-SVD. Thus, it is possible to conclude that factors $(\hat{\mathbf{G}}_1, \hat{\mathcal{G}}_2, \hat{\mathcal{G}}_3, \hat{\mathbf{G}}_4)$ comprise a valid decomposition of the original tensor \mathcal{X} .

```
# ==== SCRIPT ====
                    # -- Case 1: Generating {\mathcal X} from factors (G_1, {\mathcal G}_2, {\mathcal G}_3, G_4) --
                   # Randomly generates the TT factors and computes the tensor \mathcal{X} = G_1 ×1 \mathcal{G}_2 ×1 \mathcal{G}_3 ×1 G_4
                   R = [4 \ 3 \ 4]; # Ranks used for the decomposition
                    {\tt G_1 = randn(5,R[1]); \ \mathcal{G}_2 = randn(R[1],5,R[2]); \ \mathcal{G}_3 = randn(R[2],5,R[3]); \ {\tt G_4 = randn(R[3],5); \ \mathcal{G}_{1} = randn(R[3],5); \ \mathcal{G}_{2} = randn(R[3],5); \ \mathcal{G}_{3} = randn(R[3],5); \ \mathcal{G}_{4} = randn(R[3],5); \ \mathcal{G}_{5} = randn(R[3],5); \ \mathcal{G}_{7} = randn(R[3],5); \ \mathcal{G}_{8} = randn(R[3],5); \ \mathcal{G}_{8} = randn(R[3],5); \ \mathcal{G}_{9} = randn(R[3],5); 
    6
                    \mathcal{X} = \times^{\mathbf{1}}(G_1, G_2, G_3, G_4);
                   G_{1-}, G_{2-}, G_{3-}, G_{4-} = TTSVD(\mathcal{X});
    8
                                                                                                                                                                                               # Estimates the factors (G_1, G_2, G_3, G_4)
    9
                     @assert \mathcal{X} \approx *1(G<sub>1-</sub>, \mathcal{G}_{2-}, \mathcal{G}_{3-}, G<sub>4-</sub>)
10
                     Oshow norm(\mathcal{X} - \times^1(G_{1-}, \mathcal{G}_{2-}, \mathcal{G}_{3-}, G_{4-}))^2
11
                    # -- Case 2: Directly generating \mathcal X randomly --
13
                    \mathcal{X} = \text{randn}(5, 5, 5, 5);
14
15
                    G_{1-}, G_{2-}, G_{3-}, G_{4-} = TTSVD(\mathcal{X});
                                                                                                                                                                                                # Estimates the factors (G_1, G_2, G_3, G_4)
16
17
18
                     @assert \mathcal{X} \approx \mathsf{x^1}(\mathsf{G}_{1-},\ \mathcal{G}_{2-},\ \mathcal{G}_{3-},\ \mathsf{G}_{4-})
                     Oshow norm(\mathcal{X} - \times^1(G_{1-}, \mathcal{G}_{2-}, \mathcal{G}_{3-}, G_{4-}))^2
19
20
21
                     # ====
```

Listing 2: Script used to test the TTSVD algorithm implementation.

Moreover, we verified that the resulting estimated tensors $(\hat{\mathbf{G}}_1, \hat{\mathcal{G}}_2, \hat{\mathcal{G}}_3, \hat{\mathbf{G}}_4)$ are not actually good approximations of the original factors used to generate \mathcal{X} . In fact, we have average distances of

$$\|\mathbf{G}_1 - \hat{\mathbf{G}}_1\|_F^2 = 25.1, \quad \|\mathcal{G}_2 - \hat{\mathcal{G}}_2\|_F^2 = 61.7, \quad \|\mathcal{G}_3 - \hat{\mathcal{G}}_3\|_F^2 = 62.6, \quad \|\mathbf{G}_4 - \hat{\mathbf{G}}_4\|_F^2 = 3 \cdot 10^4.$$

This result is expected, since the decomposition is not unique: is always possible to replace a pair of successive TT-cores \mathcal{G}_j and \mathcal{G}_{j+1} by $\tilde{\mathcal{G}}_j = \mathcal{G}_j \times_3^1 \mathbf{M}_j^{-1}$ and $\tilde{\mathcal{G}}_{j+1} = \mathbf{M}_j \times_2^1 \mathcal{G}_{j+1}$ without changing the resulting tensor \mathcal{X} .