Low rank approximations of tensors

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https://surakuma.github.io/courses/daamtc.html

Properties of matrix Frobenius norm for real matrices

$$||A||_F^2 = \sum_{i,j} A^2(i,j) = Trace(AA^T) = Trace(A^TA)$$

$$||A+B||_F^2 = ||A||_F^2 + ||B||_F^2 + 2\langle A, B\rangle_F$$

Here $\langle A, B\rangle_F$ is known as Frobenius inner product and defined as $\langle A, B\rangle_F = Trace(A^TB) = Trace(B^TA)$.

If Q is an orthonormal matrix then,

$$||A||_F^2 = ||QQ^TA||_F^2 + ||(I - QQ^T)A||_F^2,$$
$$||QC||_F = ||C||_F,$$
$$||Q^TA||_F = ||QQ^TA||_F \leq ||A||_F,$$
$$\langle A - QQ^TA, QQ^TA\rangle_F = 0.$$

Tensor norm

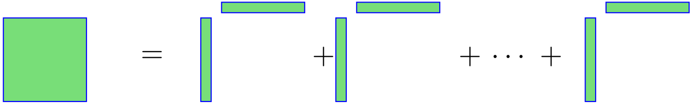
- The norm of a tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$ is analogous to the matrix Frobenius norm, and defined as

$$||\mathcal{A}||_F = \sqrt{\sum_{i_1=1}^{n_1} \sum_{i_2=1}^{n_2} \cdots \sum_{i_d=1}^{n_d} \mathcal{A}^2(i_1, i_2, \cdots, i_d)}$$

We will only focus on Frobenius norm in this course.

Singular Value Decomposition (SVD)

- It decomposes a matrix $A \in \mathbb{R}^{m \times n}$ to the form $U \Sigma V^T$
  - U is an $m \times m$ orthogonal matrix
  - V is an $n \times n$ orthogonal matrix
  - Σ is an $m \times n$ rectangular diagonal matrix
- The diagonal entries $\sigma_i = \Sigma_{ii}$ of Σ are called singular values
  - $\sigma_i \geq 0$ and $\sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_{\min(m,n)}$
- The largest r such that $\sigma_r \neq 0$ is called the rank of the matrix
- SVD represents a matrix as the sum of r rank one matrices



Low rank approximations of matrices using SVD

SVD decomposition: $A = U\Sigma V^T$

Let u_i and v_i be the column vectors of U and V, respectively.

r'-rank approximation

If $\tilde{A} = \sum_{i=1}^{r'} \sigma_i u_i v_i^T$, then $\tilde{A}$ is an r'-rank approximation of A.

$$||A - \tilde{A}||_F^2 = \sum_{i=r'+1}^{\min(m,n)} \sigma_i^2$$

SVD gives the best r'-rank approximation of any matrix.

Approximation for ϵ accuracy

We select minimum r' such that $\sum_{i=r'+1}^{\min(m,n)} \sigma_i^2 \leq \epsilon^2$. The approximation is $\tilde{A} = \sum_{i=1}^{r'} \sigma_i u_i v_i^T$.

$$||A - \tilde{A}||_F^2 = \sum_{i=r'+1}^{\min(m,n)} \sigma_i^2 \leq \epsilon^2$$

Properties of SVD

The SVD of $A \in \mathbb{R}^{m\times n}$ can be written as $A = U\Sigma V^T$. Here $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are orthogonal matrices and $\Sigma \in \mathbb{R}^{m\times n}$ is a rectangular diagonal matrix.

- Columns of U are also eigen vectors of AA^T
- Similarly, columns of V are eigen vectors of A^TA
- If $\sigma_i > 0$ is a singular value of A then σ_i^2 is an eigen value of AA^T and A^TA

$\Sigma\Sigma^T$ and $\Sigma^T\Sigma$ are diagonal matrices. Their diagonal entries are the eigen values of AA^T and A^TA, respectively.

We can also express SVD as

$$A = \begin{pmatrix} U_1 & U_2 \end{pmatrix} \begin{pmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{pmatrix} \begin{pmatrix} V_1 V_2 \end{pmatrix}^T = U_1\Sigma_1 V_1^T + U_2\Sigma_2 V_2^T.$$

This is equivalent to

$$A = U_1U_1^TA + U_2U_2^TA = AV_1V_1^T + AV_2V_2^T.$$

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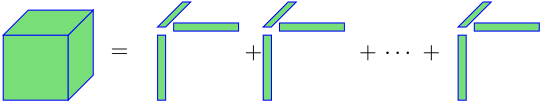
CP decomposition of $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$

It factorizes a tensor into a sum of rank one tensors.



CP decomposition of a 3-dimensional tensor.

$$\mathcal{A} = \sum_{\alpha=1}^{r} U_1(:,\alpha) \circ U_2(:,\alpha) \circ \cdots \circ U_d(:,\alpha)$$

It can be concisely expressed as $\mathcal{A} = [\![U_1, U_2, \cdots, U_d]\!]$. CP decomposition for a 3-dimensional tensor in matricized form can be written as:

$$A_{(1)} = U_1(U_3 \odot U_2)^T,\ A_{(2)} = U_2(U_3 \odot U_1)^T\ A_{(3)} = U_3(U_2 \odot U_1)^T.$$

It is useful to assume that $U_1, U_2 \cdots U_d$ are normalized to length one with the weights given in a vector $\lambda \in \mathbb{R}^r$.

$$\mathcal{A} = [\![\lambda; U_1, U_2, \cdots, U_d]\!] = \sum_{\alpha=1}^{r} \lambda_\alpha U_1(:,\alpha) \circ U_2(:,\alpha) \circ \cdots \circ U_d(:,\alpha)$$

Tensor rank

$$\mathcal{A} = \sum_{\alpha=1}^{r} \lambda_\alpha U_1(:,\alpha) \circ U_2(:,\alpha) \circ \cdots \circ U_d(:,\alpha)$$

- The minimum r required to express $\mathcal{A}$ is called the rank of $\mathcal{A}$

The rank of a real-valued tensor may be different over $\mathbb{R}$ and $\mathbb{C}$. For example, consider the frontal slices of $\mathcal{A} \in \mathbb{R}^{2\times 2\times 2}$

$$\mathcal{A}(:,:,1) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \mathcal{A}(:,:,2) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.$$

This has rank three over $\mathbb{R}$ and two over $\mathbb{C}$. The CP decomposition over $\mathbb{R}$ has the following factor matrices:

$$U_1 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & -1 \end{pmatrix}, U_2 = \begin{pmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}, \text{ and } U_3 = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 1 \end{pmatrix}.$$

The CP decomposition over $\mathbb{C}$ has the following factor matrices:

$$U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}, U_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}, \text{ and } U_3 = \begin{pmatrix} 1 & 1 \\ i & -i \end{pmatrix}.$$

Rank and low-rank approximations

- Determining the rank of a tensor is an NP-complete problem

- If $\mathcal{A} = \sum_{\alpha=1}^{r} \lambda_\alpha U_1(:,\alpha) \circ U_2(:,\alpha) \circ \cdots \circ U_d(:,\alpha)$, summing $k < r$ terms may not yield a best rank-k approximation

- Possible that the best rank-k approximation of a tensor may not exist

CP decomposition: example

Let $\mathcal{A} \in \mathbb{R}^{2\times4\times3}$ and $A = [\![U_1, U_2, U_3]\!]$. The rank of $\mathcal{A}$ is 2.

$$U_1 = \begin{pmatrix} 1 & 3 \\ 2 & 4 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 4 & 6 \\ 3 & 7 \end{pmatrix}, \quad U_3 = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}$$

Computation of $\mathcal{A}(2,3,1)$,

$$\begin{aligned} \mathcal{A}(2,3,1) =& \sum_{\alpha=1}^{2} U_1(2,\alpha)U_2(3,\alpha)U_3(1,\alpha) \\ =& 2\cdot4\cdot1 + 4\cdot6\cdot4 = 104 \end{aligned}$$

$\mathcal{A}$ has total 24 elements, while the CP representation has 18 elements.

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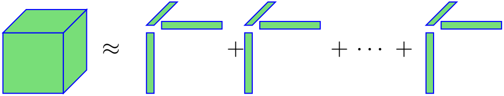
CP optimization problem for a 3-dimensional tensor



For fixed rank k, we want to solve

$$\min_{U_1, U_2 U_3} ||\mathcal{A} - \sum_{\alpha=1}^{k} \lambda_\alpha U_1(:,\alpha) \circ U_2(:,\alpha) \circ U_3(:,\alpha)||_F.$$

- It is a nonlinear, nonconvex optimization problem
- In the matrix case, the SVD provides us the optimal solution
- In the tensor case, convergence to optimum not guaranteed

Alternating Least Squares (ALS) method

Fixing all but one factor matrix, we have a linear least squares problem:

$$\min_{\hat{U}_1} ||\mathcal{A} - \sum_{\alpha=1}^{k} \hat{U}_1(:,\alpha) \circ U_2(:,\alpha) \circ U_3(:,\alpha)||_F$$

or equivalently

$$\min_{\hat{U}_1} ||A_{(1)} - \hat{U}_1(U_3 \odot U_2)^T||_F$$

ALS works by alternating over factor matrices, updating one at a time.

CP-ALS algorithm

Repeat until maximum iterations reached or no further improvement obtained

1. Solve $U_1(U_3 \odot U_2)^T = A_{(1)}$ for $U_1 \Rightarrow U_1 = A_{(1)}(U_3 \odot U_2)(U_3^T U_3 * U_2^T U_2)^\dagger$
2. Normalize columns of U_1
3. Solve $U_2(U_3 \odot U_1)^T = A_{(2)}$ for $U_2 \Rightarrow U_2 = A_{(2)}(U_3 \odot U_1)(U_3^T U_3 * U_1^T U_1)^\dagger$
4. Normalize columns of U_2
5. Solve $U_3(U_2 \odot U_1)^T = A_{(3)}$ for $U_3 \Rightarrow U_3 = A_{(3)}(U_2 \odot U_1)(U_2^T U_2 * U_1^T U_1)^\dagger$
6. Normalize columns of U_3

Here $A^\dagger$ denotes the Moore–Penrose pseudoinverse of A. We use the following identity to get expressions for U_1, U_2 and U_3:

$$(A \odot B)^T(A \odot B) = A^T A * B^T B$$

ALS for computing a CP decomposition

Algorithm 1 CP-ALS method to compute CP decomposition

Require: input tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, desired rank k, initial factor matrices $U_j \in \mathbb{R}^{n_j \times k}$ for $1 \leq j \leq d$

Ensure: $[\![\lambda; U_1, \cdots, U_d]\!]$: a rank-k CP decomposition of $\mathcal{A}$

repeat

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

    $V \leftarrow U_1^\top U_1 * \cdots * U_{i-1}^\top U_{i-1} U_{i+1}^\top U_{i+1} * \cdots * U_d^\top U_d$

    $U_i \leftarrow A_{(i)}(U_d \odot \cdots \odot U_{i+1} \odot U_{i-1} \odot U_1)$

    $U_i \leftarrow U_i V^\dagger$

    $\lambda \leftarrow$ normalize colums of U_i

  end for

until converge or the maximum number of iterations

- The collective operation $A_{(i)}(U_d \odot \cdots \odot U_{i+1} \odot U_{i-1} \odot U_1)$ is known as Matricized tensor times Khatri-Rao product (MTTKRP) computation
- U_j can be chosen randomly or by setting k left singular vectors of $A_{(j)}$ for $1 \leq j \leq d$

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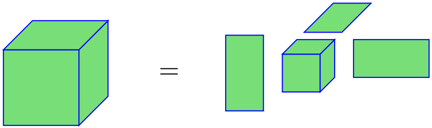
Tucker decomposition of $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$

It represents a tensor with d matrices (usually orthonormal) and a small core tensor.



Tucker decomposition of a 3-dimensional tensor.

$$\mathcal{A} = \mathcal{G} \times_1 U_1 \cdots \times_d U_d$$

$$\mathcal{A}(i_1, \cdots, i_d) = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_d=1}^{r_d} \mathcal{G}(\alpha_1, \cdots, \alpha_d) U_1(i_1, \alpha_1) \cdots U_d(i_d, \alpha_d)$$

It can be concisely expressed as $\mathcal{A} = [\![\mathcal{G}; U_1, \cdots, U_d]\!]$.

Here r_j for $1 \leq j \leq d$ denote a set of ranks. Matrices $U_j \in \mathbb{R}^{n_j \times r_j}$ for $1 \leq j \leq d$ are usually orthonormal and known as factor matrices. The tensor $\mathcal{G} \in \mathbb{R}^{r_1 \times r_2 \times \cdots \times r_d}$ is called the core tensor.

Tucker decomposition: an example

Let $\mathcal{A} \in \mathbb{R}^{3\times3\times3}$, $\mathcal{G} \in \mathbb{R}^{2\times2\times2}$ and $\mathcal{A} = [\![\mathcal{G}; U_1, U_2, U_3]\!]$.

$$U_1 = \frac{1}{3}\begin{pmatrix} 2 & -2 \\ 1 & 2 \\ 2 & 1 \end{pmatrix}, \quad U_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad U_3 = \frac{1}{5}\begin{pmatrix} 0 & 4 \\ 3 & 3 \\ 4 & 0 \end{pmatrix}$$

$$\mathcal{G}(:,:,1) = \begin{pmatrix} 1 & 4 \\ 2 & 5 \\ 3 & 6 \end{pmatrix}, \qquad \mathcal{G}(:,:,2) = \begin{pmatrix} 7 & 10 \\ 8 & 11 \\ 9 & 12 \end{pmatrix}$$

$$\begin{aligned}
\mathcal{A}(3,2,1) = &\sum_{\alpha_1=1}^{2}\sum_{\alpha_2=1}^{2}\sum_{\alpha_3=1}^{2} \mathcal{G}(\alpha_1,\alpha_2,\alpha_3)U_1(3,\alpha_1)U_2(2,\alpha_2)U_3(1,\alpha_3) \\
= &\mathcal{G}(1,1,1)U_1(3,1)U_2(2,1)U_3(1,1) + \mathcal{G}(1,1,2)U_1(3,1)U_2(2,1)U_3(1,2) \\
&+ \mathcal{G}(1,2,1)U_1(3,1)U_2(2,2)U_3(1,1) + \mathcal{G}(1,2,2)U_1(3,1)U_2(2,2)U_3(1,2) \\
&+ \mathcal{G}(2,1,1)U_1(3,2)U_2(2,1)U_3(1,1) + \mathcal{G}(2,1,2)U_1(3,2)U_2(2,1)U_3(1,2) \\
&+ \mathcal{G}(2,2,1)U_1(3,2)U_2(2,2)U_3(1,1) + \mathcal{G}(2,2,2)U_1(3,2)U_2(2,2)U_3(1,2) \\
= &1\cdot\frac{2}{3}\cdot 0\cdot 0 + 7\cdot\frac{2}{3}\cdot 0\cdot\frac{4}{5} + 4\cdot\frac{2}{3}\cdot 1\cdot 0 + 10\cdot\frac{2}{3}\cdot 1\cdot\frac{4}{5} \\
&+ 2\cdot\frac{1}{3}\cdot 0\cdot 0 + 8\cdot\frac{1}{3}\cdot 0\cdot\frac{4}{5} + 5\cdot\frac{1}{3}\cdot 1\cdot 0 + 11\cdot\frac{1}{3}\cdot 1\cdot\frac{4}{5} = \frac{124}{15}.
\end{aligned}$$

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High Order SVD (HOSVD) for computing a Tucker decomposition

Algorithm 2 HOSVD method to compute a Tucker decomposition

Require: input tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, desired rank $(r_1, \cdots, r_d)$
Ensure: $\mathcal{A} = \mathcal{G} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d$
for $k = 1$ to d **do**
  $U_k \leftarrow r_k$ leading left singular vectors of $A_{(k)}$
end for
$\mathcal{G} = \mathcal{A} \times_1 U_1^{\mathsf{T}} \times_2 U_2^{\mathsf{T}} \cdots \times_d U_d^{\mathsf{T}}$

- When $r_i < rank(A_{(i)})$ for one or more i, the decomposition is called the truncated-HOSVD (T-HOSVD)
- Output of T-HOSVD can be used as a starting point for an ALS algorithm
- The collective operation $\mathcal{A} \times_1 U_1^{\mathsf{T}} \times_2 U_2^{\mathsf{T}} \cdots \times_d U_d^{\mathsf{T}}$ is known as Multiple Tensor-Times-Matrix (Multi-TTM) computation

Quasi-optimality of T-HOSVD

Let $\tilde{\mathcal{A}} = \mathcal{G} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d$ be the tensor obtained from T-HOSVD.

$$
\begin{aligned}
||\mathcal{A} - \tilde{\mathcal{A}}||_F^2 =& ||\mathcal{A} - \mathcal{G} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d||_F^2 = ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F^2 \\
=& ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T + \mathcal{A} \times_1 U_1 U_1^T - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F^2 \\
=& ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T||_F^2 + ||\mathcal{A} \times_1 U_1 U_1^T - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F^2 \\
=& ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T||_F^2 + ||\mathcal{A} \times_1 U_1 U_1^T - \mathcal{A} \times_1 U_1 U_1^T \times_2 U_2 U_2^T||_F^2 + \cdots \\
& \cdots + ||\mathcal{A} \times_1 U_1 U_1^T \cdots \times_{d-1} U_{d-1} U_{d-1}^T - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F^2 \\
\leq& ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T||_F^2 + ||\mathcal{A} - \mathcal{A} \times_2 U_2 U_2^T||_F^2 + \cdots + ||\mathcal{A} - \mathcal{A} \times_d U_d U_d^T||_F^2
\end{aligned}
$$

Theorem

Tensor $\tilde{\mathcal{A}}$ obtained from T-HOSVD satisfies quasi-optimality condition

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

where $\mathcal{A}_{best}$ is the best approximation of $\mathcal{A}$ with ranks $(r_1, \cdots, r_d)$.

Proof: $||\mathcal{A} - \mathcal{A} \times_i U_i U_i^T||_F \leq ||\mathcal{A} - \mathcal{A}_{best}||_F$ for $1 \leq i \leq d$. Substituting these in the previous result yields the specified inequality.

Sequentially T-HOSVD (ST-HOSVD) for Tucker decomposition

- This method is more work efficient than T-HOSVD
- In each step, it reduces the size of one dimension of the tensor

Algorithm 3 ST-HOSVD method to compute a Tucker decomposition

Require: input tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, desired rank $(r_1, \cdots, r_d)$
Ensure: $[\![\mathcal{G}; U_1, \cdots, U_d]\!]$: a $(r_1, \cdots, r_d)$-rank Tucker decomposition of $\mathcal{A}$

  $\mathcal{B} \leftarrow \mathcal{A}$
  for $k = 1$ to d **do**
    $S \leftarrow B_{(k)} B_{(k)}^T$
    $U_k \leftarrow r_k$ leading eigen vectors of S
    $\mathcal{B} \leftarrow \mathcal{B} \times_k U_k$
  end for
  $\mathcal{G} = \mathcal{B}$

Quasi-optimality of ST-HOSVD

Let $\tilde{\mathcal{A}} = \mathcal{G} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d$ be the tensor obtained from ST-HOSVD.

$$\begin{aligned}||\mathcal{A} - \tilde{\mathcal{A}}||_F^2 =& ||\mathcal{A} - \mathcal{G} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d||_F^2 = ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F^2 \\ =& ||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T||_F^2 + ||\mathcal{A} \times_1 U_1 U_1^T - \mathcal{A} \times_1 U_1 U_1^T \times_2 U_2 U_2^T||_F^2 + \cdots \\ & \cdots + ||\mathcal{A} \times_1 U_1 U_1^T \cdots \times_{d-1} U_{d-1} U_{d-1}^T - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F^2\end{aligned}$$

Theorem

Tensor $\tilde{\mathcal{A}}$ obtained from ST-HOSVD satisfies quasi-optimality condition

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

where $\mathcal{A}_{best}$ is the best approximation of $\mathcal{A}$ with ranks $(r_1, \cdots, r_d)$.

Proof: We know that $||\mathcal{A} - \mathcal{A} \times_i U_i U_i^T||_F \leq ||\mathcal{A} - \mathcal{A}_{best}||_F$ for $1 \leq i \leq d$.

$$||\mathcal{A} - \mathcal{A} \times_1 U_1 U_1^T||_F \leq ||\mathcal{A} - \mathcal{A}_{best}||_F$$

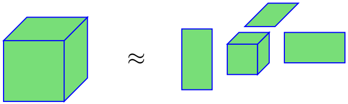
$$||\mathcal{A} \times_1 U_1 U_1^T - \mathcal{A} \times_1 U_1 U_1^T \times_2 U_2 U_2^T||_F \leq ||\mathcal{A} - \mathcal{A} \times_2 U_2 U_2^T||_F \leq ||\mathcal{A} - \mathcal{A}_{best}||_F$$

$$\vdots$$

$$||\mathcal{A} \times_1 U_1 U_1^T \cdots \times_{d-1} U_{d-1} U_{d-1}^T - \mathcal{A} \times_1 U_1 U_1^T \cdots \times_d U_d U_d^T||_F \leq ||\mathcal{A} - \mathcal{A} \times_d U_d U_d^T||_F \leq ||\mathcal{A} - \mathcal{A}_{best}||_F$$

Summing the above terms yields the specified inequality.

Tucker decomposition optimization problem for a 3-dimensional tensor



For fixed ranks orthonormal matrices U_1, U_2, U_3, we want to solve

$$\min_{U_1,U_2,U_3} ||\mathcal{A} - \mathcal{G} \times_1 U_1 \times_2 U_2 \times_3 U_3||_F, \text{ where } \mathcal{G} = \mathcal{A} \times_1 U_1^T \times_2 U_2^T \times_3 U_3^T.$$

This is equivalent to

$$\max_{U_1,U_2,U_3} ||\mathcal{A} \times_1 U_1^T \times_2 U_2^T \times_3 U_3^T||_F.$$

It is a nonlinear, nonconvex optimization problem.

Higher-order orthogonal iteration (HOOI) method

Fixing all but one factor matrix, we have a matrix problem:

$$\max_{\hat{U}_1} ||\mathcal{A} \times_1 {\hat{U}_1}^T \times_2 U_2^T \times_3 U_3^T||_F$$

HOOI works by alternating over factor matrices, updating one by computing left singular vectors

HOOI method for computing a Tucker decomposition

Algorithm 4 HOOI method to compute Tucker decomposition

Require: input tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, desired ranks $(r_1, \cdots, r_d)$, initial factor matrices $U_j \in \mathbb{R}^{n_j \times r_j}$ for $1 \leq j \leq d$

Ensure: $[\![\mathcal{G}; U_1, \cdots, U_d]\!]$: a $(r_1, \cdots, r_d)$-rank Tucker decomposition of $\mathcal{A}$

  repeat

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

      $\mathcal{B} \leftarrow \mathcal{A} \times_1 U_1^T \cdots \times_{i-1} U_{i-1}^T \times_{i+1} U_{i+1}^T \cdots \times_d U_d^T$

      $U_i \leftarrow r_i$ left singular vectors of $B_{(i)}$

    end for

  until converge or the maximum number of iterations

  $\mathcal{G} \leftarrow \mathcal{A} \times_1 U_1^T \times_2 U_2^T \cdots \times_d U_d^T$

- Outputs of HOSVD (U_j for $1 \leq j \leq d$) can be used as a starting point for this method

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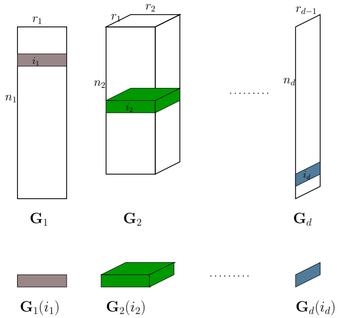
Tensor Train (TT) decomposition: Product of matrices view

- A d-dimensional tensor is represented with 2 matrices and d-2 3-dimensional tensors.



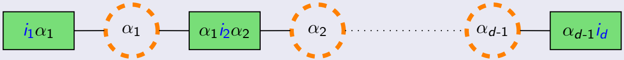
$$\mathbf{A}(i_1, i_2, \cdots, i_d) = \mathbf{G}_1(i_1)\mathbf{G}_2(i_2)\cdots\mathbf{G}_d(i_d)$$

An entry of $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ is computed by multiplying corresponding matrix (or row/column) of each matrix/tensor.

Tensor Train decomposition

$\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ is represented with cores $\mathcal{G}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$, $k=1, 2, \cdots d$, $r_0 = r_d = 1$ and its elements satisfy the following expression:

$$\mathcal{A}(i_1, \cdots, i_d) = \sum_{\alpha_0=1}^{r_0} \cdots \sum_{\alpha_d=1}^{r_d} \mathcal{G}_1(\alpha_0, i_1, \alpha_1) \cdots \mathcal{G}_d(\alpha_{d-1}, i_d, \alpha_d)$$
$$= \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} \mathcal{G}_1(1, i_1, \alpha_1) \cdots \mathcal{G}_d(\alpha_{d-1}, i_d, 1)$$



The ranks r_k are called TT-ranks.

- The number of entries in this decomposition = $\mathcal{O}(n_1 r_1 + n_2 r_1 r_2 + n_3 r_2 r_3 + \cdots + n_{d-1} r_{d-2} r_{d-1} + n_d r_{d-1})$

TT-decomposition: an example

Let $\mathcal{A} \in \mathbb{R}^{3\times4\times5}$. $\mathcal{G}_1 \in \mathbb{R}^{3\times2}, \mathcal{G}_2 \in \mathbb{R}^{2\times4\times2}$, and $\mathcal{G}_3 \in \mathbb{R}^{2\times5}$ are the cores of a TT-decomposition.

$$\mathcal{G}_1 = \begin{pmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{pmatrix}, \quad \mathcal{G}_3 = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix},$$

$$\mathcal{G}_2(:,1,:) = \begin{pmatrix} 1 & 1 \\ 2 & 1 \end{pmatrix}, \mathcal{G}_2(:,2,:) = \begin{pmatrix} 1 & 1 \\ 3 & 1 \end{pmatrix}, \mathcal{G}_2(:,3,:) = \begin{pmatrix} 1 & 1 \\ 4 & 1 \end{pmatrix}, \mathcal{G}_2(:,4,:) = \begin{pmatrix} 1 & 1 \\ 5 & 1 \end{pmatrix}$$

Computation of $\mathcal{A}(2,3,4)$,

$$\begin{aligned} \mathcal{A}(2,3,4) &= \mathcal{G}_1(2,:)\mathcal{G}_2(:,3,:)\mathcal{G}_3(:,4) \\ &= \begin{pmatrix} 2 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 4 & 1 \end{pmatrix} \begin{pmatrix} 4 \\ 1 \end{pmatrix} = 27 \end{aligned}$$

Another representation of unfolding matrices of a tensor

A_k denotes k-th unfolding matrix of tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$.

$$A_k = [A_k(i_1, i_2, \cdots, i_k; i_{k+1}, \cdots, i_d)]$$

- Size of A_k is $(\prod_{\ell=1}^{k} n_\ell) \times (\prod_{\ell=k+1}^{d} n_\ell)$

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TT-SVD algorithm for TT approximation [Oseledets, 2011]

Algorithm 5 TT-SVD algorithm

Require: d-dimensional tensor $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ and desired ranks ($r_0 = 1$, $r_1, r_2, \cdots r_{d-1}, r_d = 1$)

Ensure: Cores $\mathcal{G}_k \in \mathbb{R}^{r_{k-1} \times n_k \times r_k}$ for $1 \leq k \leq d$ of a TT representation

1: Temporary tensor: $\mathfrak{C} = \mathcal{A}$

2: **for** $k = 1 : d - 1$ **do**

3: $\quad A_k = reshape(\mathfrak{C}, r_{k-1}n_k, \frac{numel(\mathfrak{C})}{r_{k-1}n_k})$

4: $\quad$ Compute SVD: $A_k = U\Sigma V^T$

5: $\quad$ New core: $\mathcal{G}_k := reshape(U(;1 : r_k), r_{k-1}, n_k, r_k)$

6: $\quad \mathfrak{C} = \Sigma(1 : r_k; 1 : r_k)V^T(1 : r_k;)$

7: **end for**

8: $\mathcal{G}_d = \mathfrak{C}$

9: return $\mathcal{G}_1, \cdots, \mathcal{G}_d$

- $reshape(A, m_1, \cdots, m_\ell)$: rearranges array A into a $m_1 \times \cdots \times m_\ell$ array
- $numel(A)$: number of elements of array A

Error with TT-SVD approximation

Suppose the unfolding matrices of $\mathcal{A}$ satisfy the following:
$A_k = R_k + E_k, \quad R_k$ is the best r_k- rank approximation of $A_k, \quad$ for $1 \leq k \leq d-1$.

The accuracy analysis of TT-SVD is similar to that of ST-HOSVD method (see [Oseledets, 2011]).
Tensor $\mathcal{B}$ obtained from the TT-SVD algorithm satisfies

$$||\mathcal{A} - \mathcal{B}||_F^2 \leq \sum_{k=1}^{d-1} ||E_k||_F^2.$$

Theorem

Tensor $\mathcal{B}$ obtained from TT-SVD satisfies quasi-optimality condition

$$||A - \mathcal{B}||_F \leq \sqrt{d-1}||\mathcal{A} - \mathcal{A}_{best}||_F,$$

where $\mathcal{A}_{best}$ is the best $(r_1, \cdots, r_{d-1})$-ranks approximation of $\mathcal{A}$ in TT-format.

Proof: As SVD gives the best r_k rank approximation for A_k, we have

$$||E_k||_F \leq ||\mathcal{A} - \mathcal{A}_{best}||_F \text{ for } 1 \leq k \leq d.$$

Putting the values of $||E_k||_F$ in the error expression of TT-SVD algorithm completes the proof.

Why TT representation is good for high dimension tensors?

This representation allows one to perform various basic linear algebra operations in its own structure.

- *Addition*: The addition of two tensors in the TT-representation ,

$$\mathcal{A} = \mathcal{A}_1(i_1) \cdots \mathcal{A}_d(i_d), \quad \mathcal{B} = \mathcal{B}_1(i_1) \cdots \mathcal{B}_d(i_d),$$

  requires to merge cores for each mode. Auxiliary dimensions are added. The cores $\mathcal{C}_k(i_k)$ of $\mathcal{C} = \mathcal{A} + \mathcal{B}$ are defined as

$$\mathcal{C}_k(i_k) = \begin{pmatrix} \mathcal{A}_k(i_k) & 0 \\ 0 & \mathcal{B}_k(i_k) \end{pmatrix}, \quad \text{for } 2 \leq k \leq d-1, \text{ and}$$

$$\mathcal{C}_1(i_1) = \begin{pmatrix} \mathcal{A}_1(i_1) & \mathcal{B}_1(i_1) \end{pmatrix}, \quad \mathcal{C}_d(i_d) = \begin{pmatrix} \mathcal{A}_d(i_d) \\ \mathcal{B}_d(i_d) \end{pmatrix}.$$

- *Multiplication by a number*: requires to scale one of the cores
- Multidimensional contraction, Hadamard product and scalar product can also be performed
- Further approximation (or compression) can also be obtained

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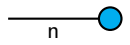
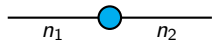
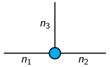
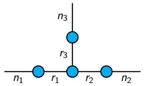
Tensor network representations

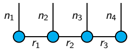
Notation: Tensors are denoted by solid shapes and number of lines denote the dimensions of the tensors. Connecting two lines implies summation (or contraction) over the connected dimensions.

Vector : 

Matrix : 

3-dimensional tensor : 

Tucker decomposition of a 3-dimensional tensor : 

TT decomposition of of a 4-dimensional tensor 

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Course project

- A list of topics/articles is given
- Each student or a group of two students will prepare a 5-6 pages report for the chosen topic/article
- Deadline for submitting the report: Nov 6
- Presentation would be after Nov 6
- Email me your or your group topic/article choices (atleast two) in preference order

If you want to propose another topic or article, your are more than welcome to discuss it with me.

Research topics

- Communication costs of a specific matrix factorization
- Use of tensors in a particular domain
  - Neuroscience, data analysis, molecular simulations, quantum computing, face recognition

What do I expect from you in the report?

- State-of-the-art of the field
- Bottleneck part of the operation
- Your idea of improvement and preliminary work on why it will be effective

Research articles

- Obtain lower bounds on data transfers for various computations on a sequential machine: Automated Derivation of Parametric Data Movement Lower Bounds for Affine Programs
- Performance optimizations for TSQR algorithm: Reconstructing Householder Vectors from Tall-Skinny QR
- Memory management in deep neural network training: Optimal GPU-CPU Offloading Strategies for Deep Neural Network Training
- Sequential lower bounds and optimal algorithms for symmetric computations: I/O-Optimal Algorithms for Symmetric Linear Algebra Kernels
- Hypergraph partitioning-based methods to improve MTTKRP performance: Scalable Sparse Tensor Decompositions in Distributed Memory Systems
- A parallel method to perform MTTKRP on a parallel shared memory machine: SPLATT: Efficient and Parallel Sparse Tensor-Matrix Multiplication
- Randomization based parallel HOSVD and ST-HOSVD methods: Parallel Randomized Tucker Decomposition Algorithms
- Tucker decomposition to improve performance of convolution kernels: Stable Low-rank Tensor Decomposition for Compression of Convolutional Neural Network
- Tensor train representation for the weight matrices of the fully connected layers: Tensorizing Neural Networks

Contents of the report for a research article

- The general idea of the work
- A detailed analysis of some parts
- Overview of the state of the art
- Mention why the work of this paper is important
- Your feedback on the work (possible extensions, limitations of the work, ...)
- What challenges you faced while reading the paper (which parts are not clear, explanation is not appropriate, missing information, ...)

Each group (or person) will do a presentation of the selected topic/article for 30-45 minutes, followed by 5-10 minutes of questions/comments.

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Main idea of randomized SVD

We want to find r-rank approximation of $A \in \mathbb{R}^{m \times n}$. We select a matrix Q with ℓ ($r \leq \ell \leq n$) orthonormal columns that well approximates the action of A, $A \approx QQ^T A$.

1. Construct $B = Q^T A$
2. Perform SVD of B, $B = \tilde{U}\Sigma V^T$
3. Set $U = Q\tilde{U}$
4. Return U, Σ, V

A simple way to find Q

1. Construct a Gaussian random matrix Ω of $n \times \ell$ size
2. Form $X = A\Omega$
3. Obtain an orthonormal matrix using QR factorization, $X = QR$

Usually $\ell - r$ is a small constant, such as 5 or 10.

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Strassen's algorithm for matrix multiplication ($C = AB$)

- Matrix is divided into 2×2 blocks

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

$$\begin{aligned}
M_1 &= (A_{11} + A_{22})(B_{11} + B_{22}) \\
M_2 &= (A_{21} + A_{22})B_{11} \\
M_3 &= A_{11}(B_{12} - B_{22}) \\
M_4 &= A_{22}(B_{21} - B_{11}) \\
M_5 &= (A_{11} + A_{12})B_{22} \\
M_6 &= (A_{21} - A_{11})(B_{11} + B_{12}) \\
M_7 &= (A_{12} - A_{22})(B_{21} + B_{22})
\end{aligned}$$

$$\begin{aligned}
C_{11} &= M_1 + M_4 - M_5 + M_7 \\
C_{12} &= M_3 + M_5 \\
C_{21} &= M_2 + M_4 \\
C_{22} &= M_1 - M_2 + M_3 + M_6
\end{aligned}$$

2×2 Matrix multiplication as a tensor operation

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

We can write this multiplication as a tensor operation,

$$\mathfrak{T} \times_1 \begin{pmatrix} A_{11} \\ A_{12} \\ A_{21} \\ A_{22} \end{pmatrix} \times_2 \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix} = \begin{pmatrix} C_{11} \\ C_{12} \\ C_{21} \\ C_{22} \end{pmatrix}$$

Where $\mathfrak{T}$ is a $4 \times 4 \times 4$ tensor with the following frontal slices:

$$T_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} T_2 = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad T_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix} T_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

2×2 Matrix multiplication as a tensor operation

$$\begin{pmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{pmatrix}$$

We can write this multiplication as a tensor operation,

$$\mathfrak{T} \times_1 \begin{pmatrix} A_{11} \\ A_{12} \\ A_{21} \\ A_{22} \end{pmatrix} \times_2 \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix} = \begin{pmatrix} C_{11} \\ C_{12} \\ C_{21} \\ C_{22} \end{pmatrix}$$

For example,

$$T_2 \times_1 \begin{pmatrix} A_{11} \\ A_{12} \\ A_{21} \\ A_{22} \end{pmatrix} \times_2 \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix} = \begin{pmatrix} A_{11} & A_{12} & A_{21} & A_{22} \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix} = A_{11}B_{12} + A_{12}B_{22} = C_{12}$$

Matrix multiplication with CP decomposition

CP decomposition of $\mathcal{T}$, $\mathcal{T} = [\![U, V, W]\!]$ can be written as,

$$\mathcal{T} = \sum_{r=1}^{R} u_r \circ v_r \circ w_r$$

Here u_r, v_r and w_r are the columns of U, V and W, respectively. R is the rank of $\mathcal{T}$. We can write matrix multiplication as,

$$\mathcal{T} \times_1 \begin{pmatrix} A_{11} \\ A_{12} \\ A_{21} \\ A_{22} \end{pmatrix} \times_2 \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix} = \sum_{r=1}^{R} (u_r \circ v_r \circ w_r) \times_1 \begin{pmatrix} A_{11} \\ A_{12} \\ A_{21} \\ A_{22} \end{pmatrix} \times_2 \begin{pmatrix} B_{11} \\ B_{12} \\ B_{21} \\ B_{22} \end{pmatrix}$$

$$= \sum_{r=1}^{R} \Big[(A_{11} \; A_{12} \; A_{21} \; A_{22}) u_r (B_{11} \; B_{12} \; B_{21} \; B_{22}) v_r \Big] w_r = \begin{pmatrix} C_{11} \\ C_{12} \\ C_{21} \\ C_{22} \end{pmatrix}$$

Factor matrices and Strassen's algorithm

Factor matrices,

$$U = \begin{pmatrix} 1 & 0 & 1 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & -1 \end{pmatrix}$$

$$V = \begin{pmatrix} 1 & 1 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 1 & 0 & -1 & 0 & 1 & 0 & 1 \end{pmatrix}$$

$$W = \begin{pmatrix} 1 & 0 & 0 & 1 & -1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 1 & -1 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Strassen's algorithm,

$$\begin{aligned} M_1 &= (A_{11} + A_{22})(B_{11} + B_{22}) \\ M_2 &= (A_{21} + A_{22})B_{11} \\ M_3 &= A_{11}(B_{12} - B_{22}) \\ M_4 &= A_{22}(B_{21} - B_{11}) \\ M_5 &= (A_{11} + A_{12})B_{22} \\ M_6 &= (A_{21} - A_{11})(B_{11} + B_{12}) \\ M_7 &= (A_{12} - A_{22})(B_{21} + B_{22}) \end{aligned}$$

$$\begin{aligned} C_{11} &= M_1 + M_4 - M_5 + M_7 \\ C_{12} &= M_3 + M_5 \\ C_{21} &= M_2 + M_4 \\ C_{22} &= M_1 - M_2 + M_3 + M_6 \end{aligned}$$

Factor matrices U, V and W construct the algorithm.