

# Low rank approximations of tensors

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

# Properties of matrix Frobenius norm for real matrices

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

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

Here  $\langle A, B \rangle_F$  is known as Frobenius inner product and defined as  $\langle A, B \rangle_F = \text{Trace}(A^T B) = \text{Trace}(B^T A)$ .

If  $Q$  is an orthonormal matrix then,

$$\|A\|_F^2 = \|QQ^T A\|_F^2 + \|(I - QQ^T)A\|_F^2,$$

$$\|QC\|_F = \|C\|_F,$$

$$\|Q^T A\|_F = \|QQ^T A\|_F \leq \|A\|_F,$$

$$\langle A - QQ^T A, QQ^T A \rangle_F = 0.$$

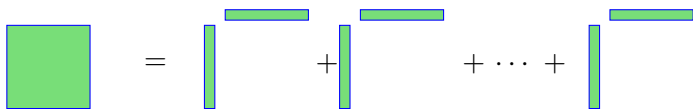
- The norm of a tensor  $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$  is analogous to the matrix Frobenius norm, and defined as

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

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
  - $\Sigma$  is an  $m \times n$  rectangular diagonal matrix
- The diagonal entries  $\sigma_i = \Sigma_{ii}$  of  $\Sigma$  are called singular values
  - $\sigma_i \geq 0$  and  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{\min(m,n)}$
- 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 $\epsilon$ 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  $A^T A$
- If  $\sigma_i > 0$  is a singular value of  $A$  then  $\sigma_i^2$  is an eigen value of  $AA^T$  and  $A^T A$

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

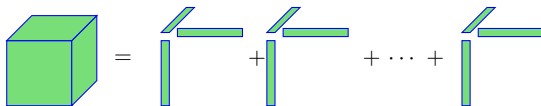
$$A = U_1 U_1^T A + U_2 U_2^T A = A V_1 V_1^T + A V_2 V_2^T.$$

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

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



CP decomposition of a 3-dimensional tensor.

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

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

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

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

$$\mathcal{A} = \llbracket \lambda; U_1, U_2, \dots, U_d \rrbracket = \sum_{\alpha=1}^r \lambda_{\alpha} U_1(:, \alpha) \circ U_2(:, \alpha) \circ \dots \circ U_d(:, \alpha)$$



# 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  $\mathcal{A} \in \mathbb{R}^{2 \times 4 \times 3}$  and  $A = \llbracket U_1, U_2, U_3 \rrbracket$ . 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  $\mathcal{A}(2, 3, 1)$ ,

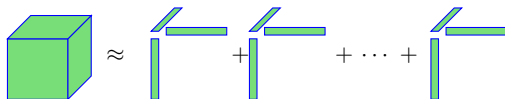
$$\begin{aligned} \mathcal{A}(2, 3, 1) &= \sum_{\alpha=1}^2 U_1(2, \alpha) U_2(3, \alpha) U_3(1, \alpha) \\ &= 2 \cdot 4 \cdot 1 + 4 \cdot 6 \cdot 4 = 104 \end{aligned}$$

$\mathcal{A}$  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

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

- 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:

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

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

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**Algorithm 1** CP-ALS method to compute CP decomposition

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

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

repeat

for  $i = 1$  to  $d$  do

$$V \leftarrow U_1^T U_1 * \dots * U_{i-1}^T U_{i-1} * U_{i+1}^T U_{i+1} * \dots * U_d^T U_d$$

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

$$U_i \leftarrow U_i V^\dagger$$

$$\lambda \leftarrow \text{normalize columns of } U_i$$

end for

**until** converge or the maximum number of iterations

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- The collective operation  $A_{(i)}(U_d \odot \dots \odot U_{i+1} \odot U_{i-1} \odot U_1)$  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  $1 \leq j \leq d$

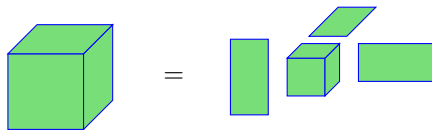


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# Tucker decomposition of $\mathcal{A} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_d}$

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



Tucker decomposition of a 3-dimensional tensor.

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

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

It can be concisely expressed as  $\mathcal{A} = \llbracket \mathcal{G}; U_1, \dots, U_d \rrbracket$ .

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

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

$$\mathcal{G}(:, :, 1) = \begin{pmatrix} 1 & 4 \\ 2 & 5 \end{pmatrix}, \quad \mathcal{G}(:, :, 2) = \begin{pmatrix} 7 & 10 \\ 8 & 11 \end{pmatrix}$$

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

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**Algorithm 2** HOSVD method to compute a Tucker decomposition

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**Require:** input tensor  $\mathcal{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ , desired rank  $(r_1, \dots, r_d)$

**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**

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

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- When  $r_i < \text{rank}(A_{(i)})$  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  $\mathcal{A} \times_1 U_1^T \times_2 U_2^T \cdots \times_d U_d^T$  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.

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

## Theorem

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

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

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

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

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## Algorithm 3 ST-HOSVD method to compute a Tucker decomposition

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**Require:** input tensor  $\mathcal{A} \in \mathbb{R}^{n_1 \times \dots \times n_d}$ , desired rank  $(r_1, \dots, r_d)$

**Ensure:**  $\llbracket \mathcal{G}; U_1, \dots, U_d \rrbracket$  : a  $(r_1, \dots, r_d)$ -rank Tucker decomposition of  $\mathcal{A}$

$\mathcal{B} \leftarrow \mathcal{A}$

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

$U_k \leftarrow r_k$  leading singular vectors of  $B_{(k)}$

$\mathcal{B} \leftarrow \mathcal{B} \times_k U_k^T$

**end for**

$\mathcal{G} = \mathcal{B}$

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# 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.

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

## Theorem

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

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

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

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

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

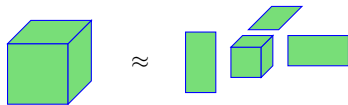
$$\|\mathcal{A} \times_1 U_1 U_1^T - \mathcal{A} \times_1 U_1 U_1^T \times_2 U_2 U_2^T\|_F \leq \|\mathcal{A} - \mathcal{A} \times_2 U_2 U_2^T\|_F \leq \|\mathcal{A} - \mathcal{A}_{\text{best}}\|_F$$

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

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.

$$\begin{aligned} \|\mathcal{A} - \mathcal{G} \times_1 U_1 \times_2 U_2 \times_3 U_3\|_F^2 &= \|\mathcal{A}\|_F^2 + \|\mathcal{G} \times_1 U_1 \times_2 U_2 \times_3 U_3\|_F^2 \\ &\quad - 2\langle \mathcal{A} - \mathcal{G} \times_1 U_1 \times_2 U_2 \times_3 U_3 \rangle \\ &= \|\mathcal{A}\|_F^2 + \|\mathcal{G}\|_F^2 - 2\langle \mathcal{A} \times_1 U_1^T \times_2 U_2^T \times_3 U_3^T, \mathcal{G} \rangle \\ &= \|\mathcal{A}\|_F^2 - \|\mathcal{G}\|_F^2 \end{aligned}$$

# 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

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**Algorithm 4** HOOI method to compute Tucker decomposition

---

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

**Ensure:**  $[\mathcal{G}; U_1, \dots, U_d]$  : a  $(r_1, \dots, r_d)$ -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

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

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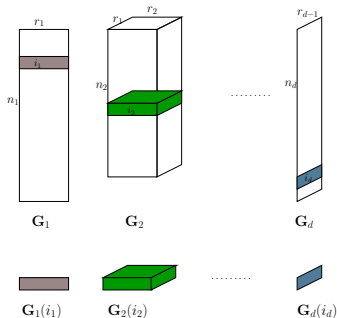
- Outputs of HOSVD ( $U_j$  for  $1 \leq j \leq d$ ) can be used as a starting point for this method

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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.



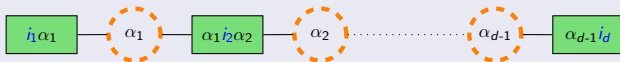
$$\mathcal{A}(i_1, i_2, \dots, i_d) = \mathbf{G}_1(i_1) \mathbf{G}_2(i_2) \cdots \mathbf{G}_d(i_d)$$

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

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

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



The ranks  $r_k$  are called TT-ranks.

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

# TT-decomposition: an example

Let  $\mathcal{A} \in \mathbb{R}^{3 \times 4 \times 5}$ .  $\mathcal{G}_1 \in \mathbb{R}^{3 \times 2}$ ,  $\mathcal{G}_2 \in \mathbb{R}^{2 \times 4 \times 2}$ , and  $\mathcal{G}_3 \in \mathbb{R}^{2 \times 5}$  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  $\mathcal{A} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ .

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

- 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]

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## Algorithm 5 TT-SVD algorithm

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

**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:  $\mathcal{C} = \mathcal{A}$
  - 2: **for**  $k = 1 : d - 1$  **do**
  - 3:      $A_k = \text{reshape}(\mathcal{C}, r_{k-1} n_k, \frac{\text{numel}(\mathcal{C})}{r_{k-1} n_k})$
  - 4:     Compute SVD:  $A_k = U \Sigma V^T$
  - 5:     New core:  $\mathcal{G}_k := \text{reshape}(U(:, 1 : r_k), r_{k-1}, n_k, r_k)$
  - 6:      $\mathcal{C} = \Sigma(1 : r_k; 1 : r_k) V^T(1 : r_k; )$
  - 7: **end for**
  - 8:  $\mathcal{G}_d = \mathcal{C}$
  - 9: return  $\mathcal{G}_1, \dots, \mathcal{G}_d$
- 

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

# Error with TT-SVD approximation

Suppose the unfolding matrices of  $\mathcal{A}$  satisfy the following:

$A_k = R_k + E_k$ ,  $R_k$  is the best  $r_k$ -rank approximation of  $A_k$ , 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

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

where  $\mathcal{A}_{best}$  is the best  $(r_1, \dots, r_{d-1})$ -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.

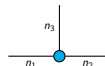
Vector :



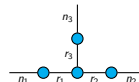
Matrix :



3-dimensional tensor :



Tucker decomposition of a 3-dimensional tensor :



TT decomposition of of a 4-dimensional tensor



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  - Strassen's algorithm: application of CP-decomposition

# 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 5
- Presentation would be after Nov 5
- Email me your or your group topic/article choices (atleast two) in preference order by Oct 15

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
- Extending a specific matrix factorization for tensors
- 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](#)
- Low rank approximation for stencil computations: [LoRAStencil: Low-Rank Adaptation of Stencil Computation on Tensor Cores](#)
- 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](#)
- Use of tensor train representation in quantum systems: [The density-matrix renormalization group: a short introduction](#)

# 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 20-35 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  $\ell$  ( $r \leq \ell \leq n$ ) 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  $U, \Sigma, V$

## A simple way to find $Q$

- 1 Construct a Gaussian random matrix  $\Omega$  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  $2 \times 2$  blocks

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

$$M_1 = (A_{11} + A_{22})(B_{11} + B_{22})$$

$$M_2 = (A_{21} + A_{22})B_{11}$$

$$M_3 = A_{11}(B_{12} - B_{22})$$

$$M_4 = A_{22}(B_{21} - B_{11})$$

$$M_5 = (A_{11} + A_{12})B_{22}$$

$$M_6 = (A_{21} - A_{11})(B_{11} + B_{12})$$

$$M_7 = (A_{12} - A_{22})(B_{21} + B_{22})$$

$$C_{11} = M_1 + M_4 - M_5 + M_7$$

$$C_{12} = M_3 + M_5$$

$$C_{21} = M_2 + M_4$$

$$C_{22} = M_1 - M_2 + M_3 + M_6$$

## $2 \times 2$ 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,

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

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

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



## $2 \times 2$ 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,

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

For example,

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

# Matrix multiplication with CP decomposition

CP decomposition of  $\mathcal{T}$ ,  $\mathcal{T} = \llbracket U, V, W \rrbracket$  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,

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

# 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,

$$M_1 = (A_{11} + A_{22})(B_{11} + B_{22})$$

$$M_2 = (A_{21} + A_{22})B_{11}$$

$$M_3 = A_{11}(B_{12} - B_{22})$$

$$M_4 = A_{22}(B_{21} - B_{11})$$

$$M_5 = (A_{11} + A_{12})B_{22}$$

$$M_6 = (A_{21} - A_{11})(B_{11} + B_{12})$$

$$M_7 = (A_{12} - A_{22})(B_{21} + B_{22})$$

$$C_{11} = M_1 + M_4 - M_5 + M_7$$

$$C_{12} = M_3 + M_5$$

$$C_{21} = M_2 + M_4$$

$$C_{22} = M_1 - M_2 + M_3 + M_6$$

Factor matrices  $U$ ,  $V$  and  $W$  construct the algorithm.